Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 05:51 AM EST

PDB ID	:	6WXU
EMDB ID	:	EMD-21963
Title	:	CryoEM structure of mouse DUOX1-DUOXA1 complex in the dimer-of-dimer state
Authors	:	Sun, J.
Deposited on	:	2020-05-12
Resolution	:	2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

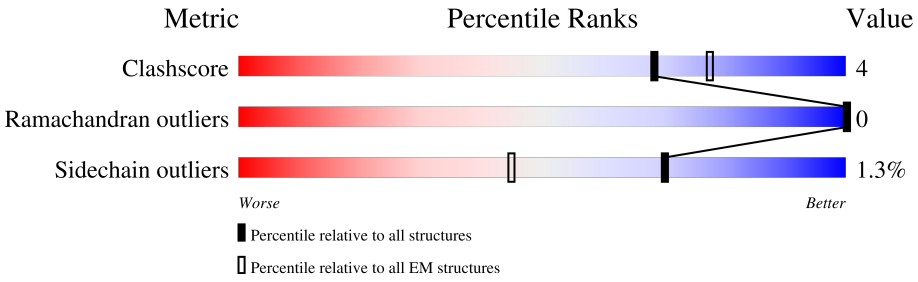
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1536	49% 6% 46%
1	C	1536	49% 6% 46%
2	B	341	73% 6% 20%
2	D	341	73% 7% 20%
3	E	11	9% 73% 18%
3	F	11	9% 73% 18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dual oxidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	834	Total 6624	C 4287	N 1151	O 1161	S 25	0	0
1	C	834	Total 6624	C 4287	N 1151	O 1161	S 25	0	0

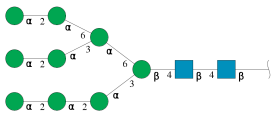
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	expression tag	UNP A2AQ92
A	17	PRO	-	expression tag	UNP A2AQ92
A	18	SER	-	expression tag	UNP A2AQ92
A	19	ARG	-	expression tag	UNP A2AQ92
C	16	GLY	-	expression tag	UNP A2AQ92
C	17	PRO	-	expression tag	UNP A2AQ92
C	18	SER	-	expression tag	UNP A2AQ92
C	19	ARG	-	expression tag	UNP A2AQ92

- Molecule 2 is a protein called Dual oxidase maturation factor 1.

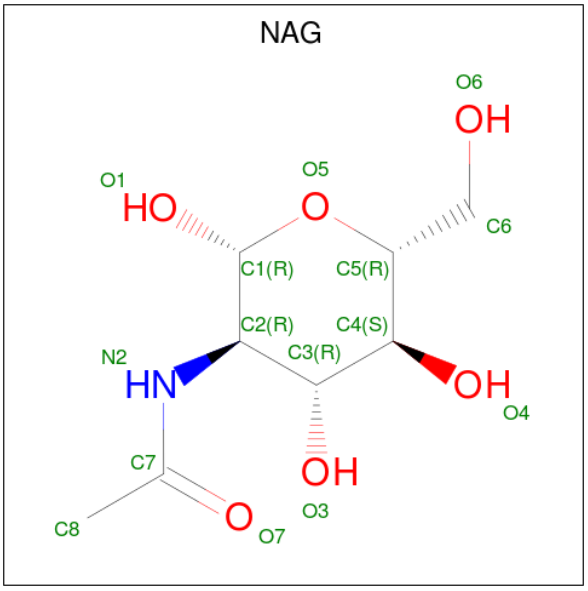
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	273	Total 2093	C 1390	N 340	O 351	S 12	0	0
2	D	273	Total 2093	C 1390	N 340	O 351	S 12	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
3	E	11	Total C N O 127 70 2 55	0	0
3	F	11	Total C N O 127 70 2 55	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 42 24 3 15	0
4	A	1	Total C N O 42 24 3 15	0
4	A	1	Total C N O 42 24 3 15	0
4	B	1	Total C N O 28 16 2 10	0
4	B	1	Total C N O 28 16 2 10	0
4	C	1	Total C N O 42 24 3 15	0
4	C	1	Total C N O 42 24 3 15	0

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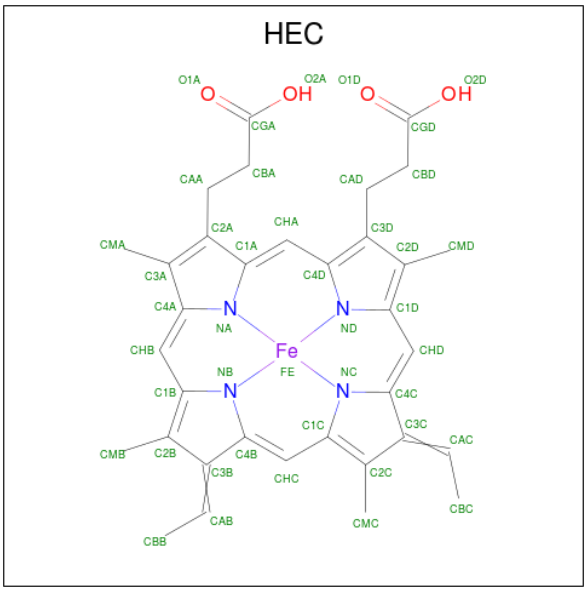
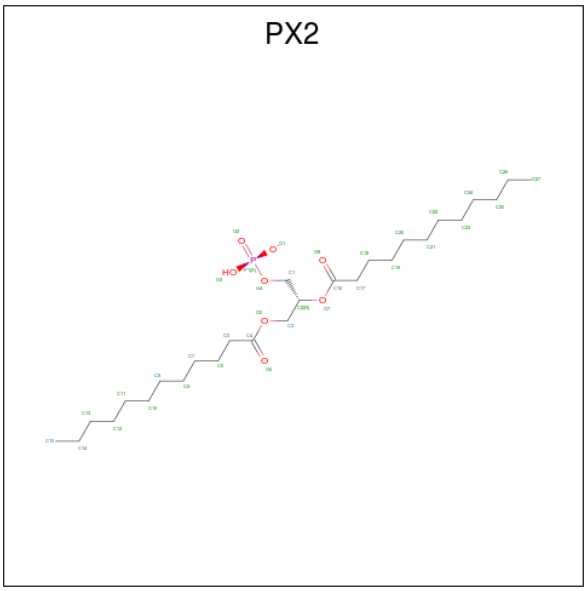
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			42	24	3	15	
4	D	1	Total	C	N	O	0
			28	16	2	10	
4	D	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



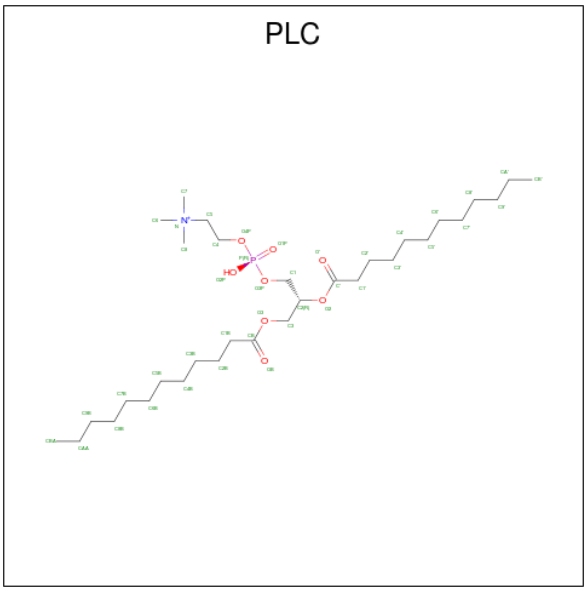
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
5	A	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
5	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
5	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 6 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: $C_{27}H_{52}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			36	27	8	1	
6	C	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 7 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			42	32	1	8	1	

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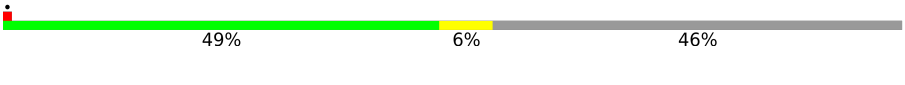
Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

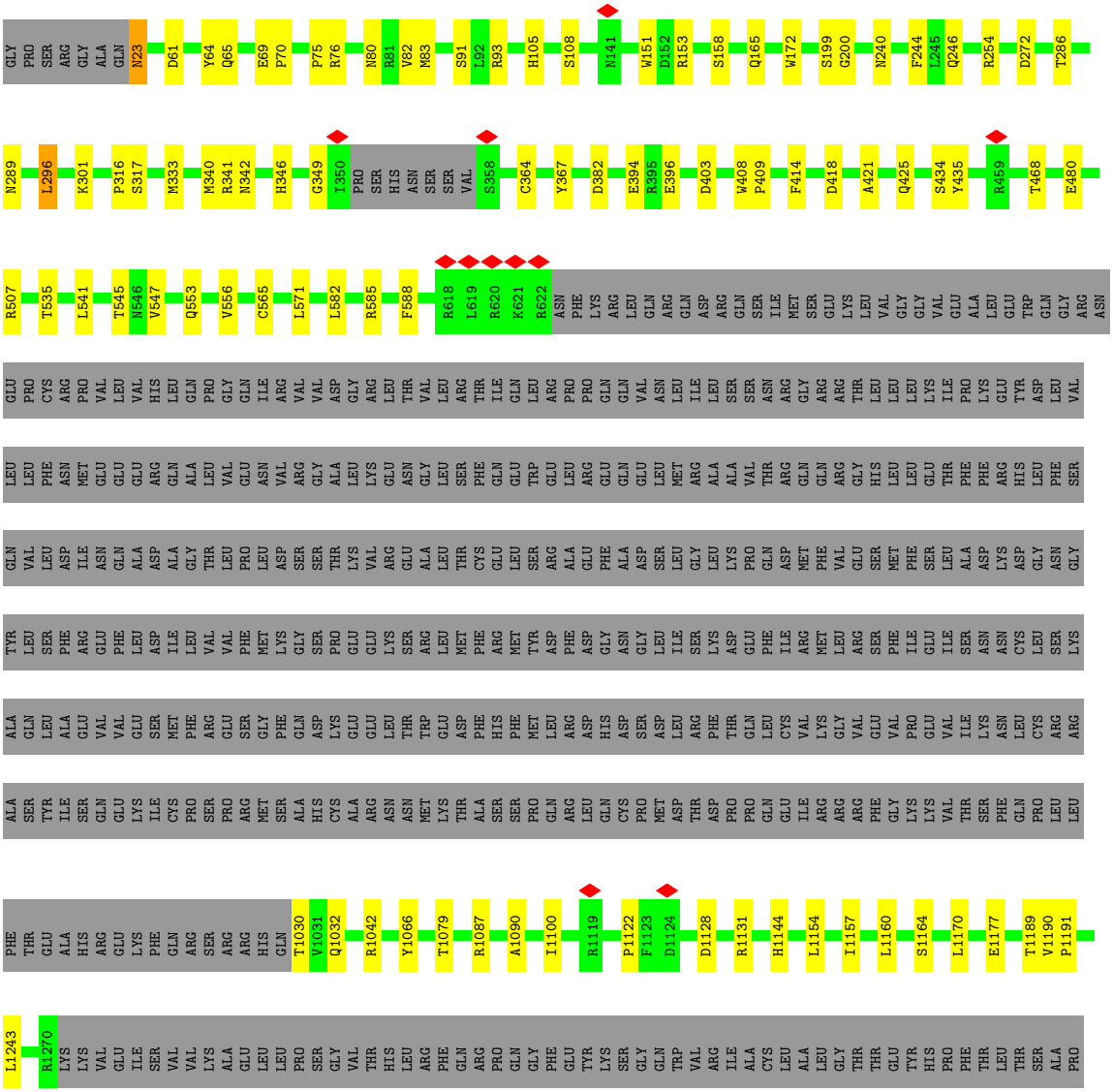
3 Residue-property plots (i)

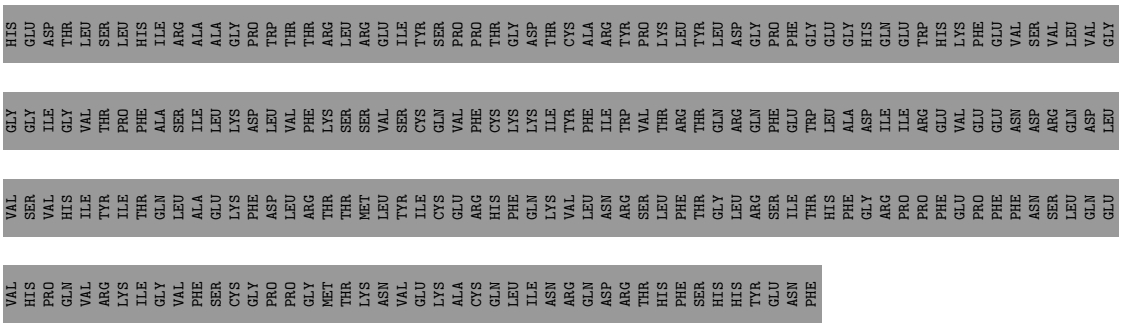
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dual oxidase 1

Chain A:

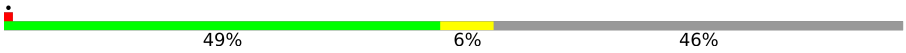


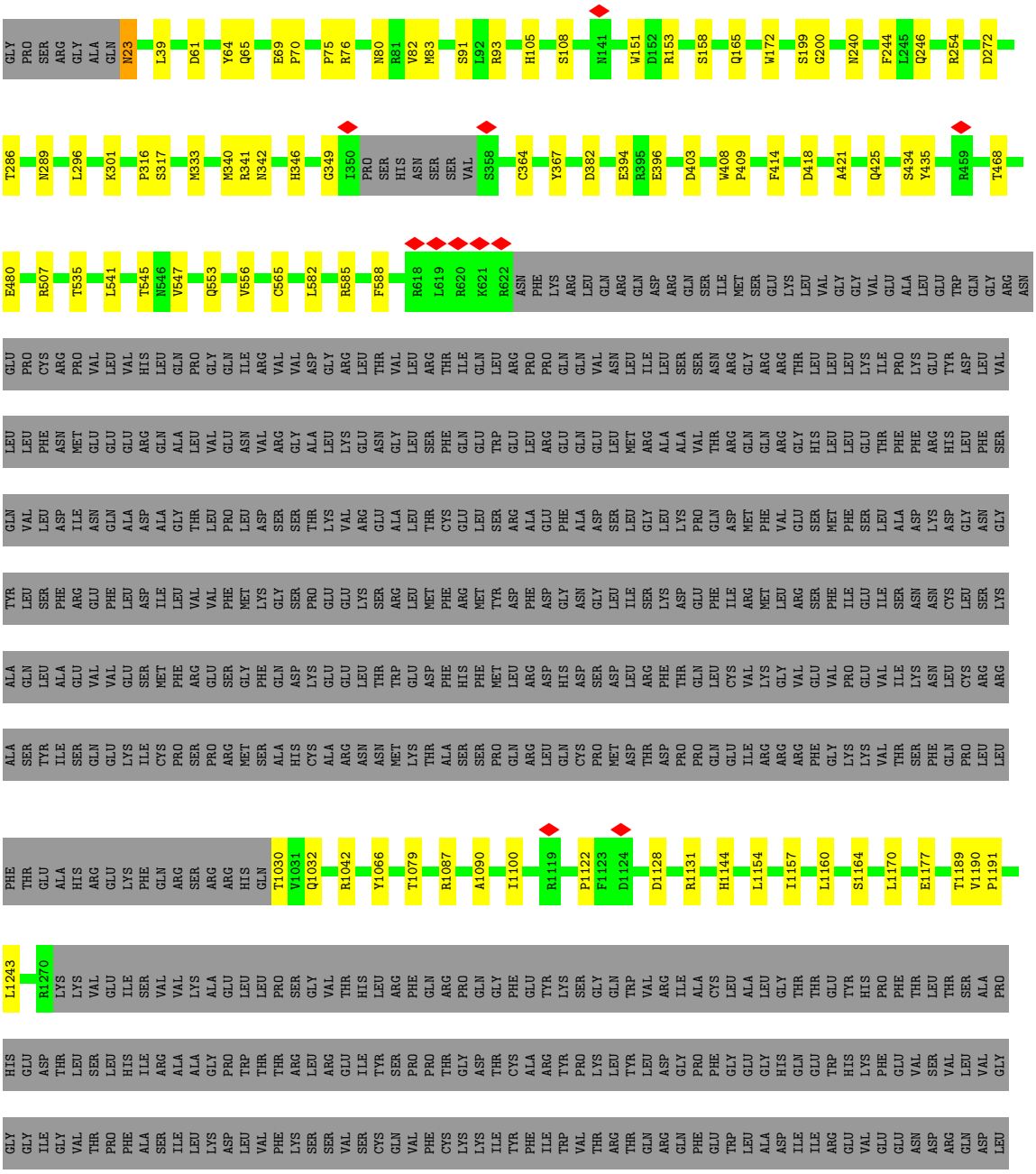


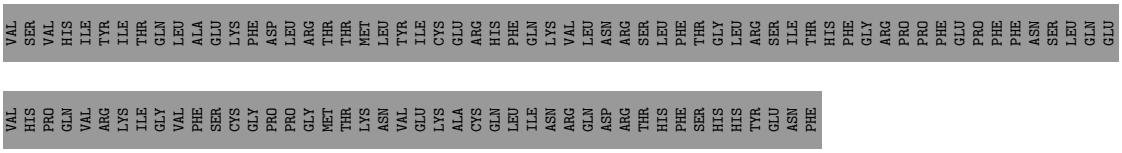


• Molecule 1: Dual oxidase 1

Chain C:

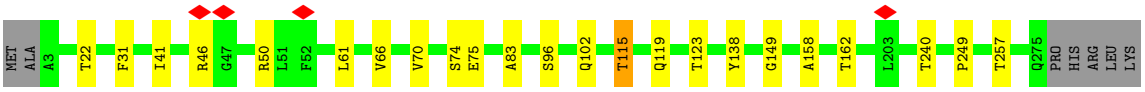






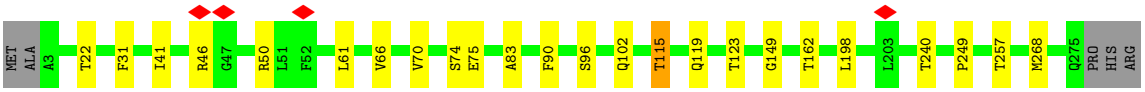
• Molecule 2: Dual oxidase maturation factor 1

Chain B:



• Molecule 2: Dual oxidase maturation factor 1

Chain D:



• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	302097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.303	Depositor
Minimum map value	-2.021	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	248.40001, 248.40001, 248.40001	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, PLC, PX2, HEC, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/6830	0.46	1/9301 (0.0%)
1	C	0.37	0/6830	0.46	1/9301 (0.0%)
2	B	0.34	0/2154	0.44	0/2950
2	D	0.34	0/2154	0.44	0/2950
All	All	0.37	0/17968	0.45	2/24502 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1128	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	1128	ASP	CB-CG-OD2	5.21	122.98	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	115	THR	Peptide
2	D	115	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6624	0	6436	53	0
1	C	6624	0	6436	52	0
2	B	2093	0	2125	12	0
2	D	2093	0	2125	13	0
3	E	127	0	106	2	0
3	F	127	0	106	2	0
4	A	42	0	39	1	0
4	B	28	0	26	1	0
4	C	42	0	39	1	0
4	D	28	0	26	1	0
5	A	86	0	64	7	0
5	C	86	0	64	7	0
6	A	36	0	52	1	0
6	C	36	0	52	1	0
7	B	42	0	64	2	0
7	D	42	0	64	2	0
All	All	18156	0	17824	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:THR:OG1	7:D:414:PLC:H62	1.84	0.78
2:B:22:THR:OG1	7:B:414:PLC:H62	1.84	0.77
7:D:414:PLC:H63	3:F:2:NAG:H2	1.68	0.76
1:C:151:TRP:O	1:C:153:ARG:NH1	2.19	0.76
7:B:414:PLC:H63	3:E:2:NAG:H2	1.68	0.75
1:A:151:TRP:O	1:A:153:ARG:NH1	2.19	0.74
1:A:82:VAL:HG23	1:A:83:MET:HG3	1.72	0.72
1:A:1100:ILE:HG21	5:A:1604:HEC:HBC2	1.72	0.71
1:A:76:ARG:NH1	1:A:418:ASP:OD2	2.23	0.71
1:C:82:VAL:HG23	1:C:83:MET:HG3	1.72	0.71
1:C:76:ARG:NH1	1:C:418:ASP:OD2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:ILE:HG21	5:C:1604:HEC:HBC2	1.72	0.70
1:A:76:ARG:O	1:A:80:ASN:ND2	2.26	0.68
1:C:342:ASN:HB2	1:C:346:HIS:HB3	1.76	0.68
1:A:1079:THR:HG22	1:A:1154:LEU:HD12	1.76	0.68
1:A:342:ASN:HB2	1:A:346:HIS:HB3	1.76	0.68
2:D:66:VAL:HG11	2:D:257:THR:HG21	1.75	0.68
2:B:66:VAL:HG11	2:B:257:THR:HG21	1.75	0.68
1:C:76:ARG:O	1:C:80:ASN:ND2	2.26	0.68
1:C:1079:THR:HG22	1:C:1154:LEU:HD12	1.76	0.68
1:C:341:ARG:NH1	1:C:565:CYS:SG	2.68	0.67
1:A:341:ARG:NH1	1:A:565:CYS:SG	2.68	0.67
1:A:254:ARG:NH2	1:A:382:ASP:OD1	2.31	0.63
4:A:1603:NAG:H3	4:A:1603:NAG:H83	1.81	0.63
2:D:75:GLU:HB3	2:D:249:PRO:HD2	1.82	0.62
2:B:75:GLU:HB3	2:B:249:PRO:HD2	1.82	0.62
4:C:1603:NAG:H3	4:C:1603:NAG:H83	1.81	0.61
1:C:254:ARG:NH2	1:C:382:ASP:OD1	2.31	0.61
5:A:1604:HEC:HMB1	5:A:1604:HEC:HBB2	1.81	0.61
5:C:1604:HEC:HMB1	5:C:1604:HEC:HBB2	1.81	0.60
1:A:240:ASN:OD1	1:A:246:GLN:NE2	2.32	0.60
1:A:1170:LEU:HD22	1:A:1243:LEU:HD11	1.83	0.60
1:A:1131:ARG:HH11	1:A:1131:ARG:CB	2.14	0.60
1:C:1131:ARG:HH11	1:C:1131:ARG:CB	2.14	0.59
1:C:1170:LEU:HD22	1:C:1243:LEU:HD11	1.83	0.59
5:C:1605:HEC:HBB2	5:C:1605:HEC:HMB1	1.84	0.59
5:A:1605:HEC:HMB1	5:A:1605:HEC:HBB2	1.83	0.59
1:C:240:ASN:OD1	1:C:246:GLN:NE2	2.32	0.59
1:A:585:ARG:NH1	1:A:1177:GLU:OE2	2.36	0.59
1:C:585:ARG:NH1	1:C:1177:GLU:OE2	2.36	0.58
1:C:1131:ARG:HH11	1:C:1131:ARG:HB3	1.69	0.58
1:A:151:TRP:HA	1:A:165:GLN:HA	1.88	0.56
1:A:1131:ARG:HH11	1:A:1131:ARG:HB3	1.69	0.56
1:C:91:SER:OG	1:C:396:GLU:OE2	2.23	0.56
1:A:91:SER:OG	1:A:396:GLU:OE2	2.23	0.56
1:C:151:TRP:HA	1:C:165:GLN:HA	1.88	0.55
2:B:83:ALA:HA	4:B:401:NAG:H82	1.89	0.55
1:C:23:ASN:N	1:C:23:ASN:OD1	2.40	0.55
2:B:41:ILE:HG23	1:C:1042:ARG:HG2	1.89	0.54
2:D:83:ALA:HA	4:D:401:NAG:H82	1.89	0.54
1:C:289:ASN:HD22	1:C:535:THR:HG22	1.73	0.54
1:A:286:THR:HG23	1:A:535:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:PHE:HB2	1:C:1157:ILE:HG22	1.90	0.54
1:A:588:PHE:HB2	1:A:1157:ILE:HG22	1.90	0.53
1:A:289:ASN:HD22	1:A:535:THR:HG22	1.73	0.53
1:A:1131:ARG:CB	1:A:1131:ARG:NH1	2.72	0.53
1:A:23:ASN:N	1:A:23:ASN:OD1	2.40	0.52
1:C:1131:ARG:CB	1:C:1131:ARG:NH1	2.72	0.52
5:C:1605:HEC:HMC1	5:C:1605:HEC:HBC3	1.91	0.52
5:A:1604:HEC:HMC1	5:A:1604:HEC:HBC3	1.92	0.52
1:A:317:SER:O	1:A:507:ARG:NH1	2.43	0.52
5:A:1605:HEC:HMC1	5:A:1605:HEC:HBC3	1.91	0.52
1:C:286:THR:HG23	1:C:535:THR:HG21	1.90	0.51
1:A:1042:ARG:HG2	2:D:41:ILE:HG23	1.93	0.51
1:C:317:SER:O	1:C:507:ARG:NH1	2.43	0.51
5:C:1604:HEC:HMC1	5:C:1604:HEC:HBC3	1.92	0.51
1:C:1122:PRO:O	6:C:1606:PX2:H41	2.12	0.50
2:D:123:THR:O	3:F:5:MAN:O3	2.26	0.49
2:B:96:SER:H	2:B:119:GLN:HE22	1.61	0.48
1:A:1122:PRO:O	6:A:1606:PX2:H41	2.12	0.48
1:A:75:PRO:HG2	1:A:425:GLN:NE2	2.29	0.48
2:D:96:SER:H	2:D:119:GLN:HE22	1.61	0.48
1:C:75:PRO:HG2	1:C:425:GLN:NE2	2.29	0.48
1:C:1131:ARG:CD	5:C:1604:HEC:HMB2	2.44	0.48
1:A:418:ASP:HB3	1:A:421:ALA:HB3	1.96	0.47
1:A:414:PHE:HD1	1:A:582:LEU:HD21	1.79	0.47
1:C:418:ASP:HB3	1:C:421:ALA:HB3	1.96	0.47
1:C:434:SER:OG	1:C:435:TYR:N	2.47	0.47
1:A:1131:ARG:CD	5:A:1604:HEC:HMB2	2.44	0.47
1:C:364:CYS:HA	1:C:367:TYR:CE2	2.49	0.47
1:C:414:PHE:HD1	1:C:582:LEU:HD21	1.79	0.47
1:A:434:SER:OG	1:A:435:TYR:N	2.47	0.47
1:A:364:CYS:HA	1:A:367:TYR:CE2	2.49	0.46
1:C:1131:ARG:NH1	1:C:1131:ARG:HB2	2.30	0.46
1:A:1131:ARG:NH1	1:A:1131:ARG:HB2	2.30	0.46
1:A:1190:VAL:HB	1:A:1191:PRO:HD3	1.96	0.46
1:C:1190:VAL:HB	1:C:1191:PRO:HD3	1.96	0.46
2:D:31:PHE:HD2	2:D:61:LEU:HG	1.82	0.45
1:C:545:THR:HG22	1:C:547:VAL:HG13	1.98	0.45
1:C:61:ASP:OD1	1:C:65:GLN:HB2	2.17	0.45
1:A:61:ASP:OD1	1:A:65:GLN:HB2	2.17	0.45
1:A:545:THR:HG22	1:A:547:VAL:HG13	1.98	0.44
1:A:333:MET:HA	1:A:394:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:PHE:HD2	2:B:61:LEU:HG	1.82	0.44
1:C:105:HIS:O	1:C:108:SER:OG	2.29	0.44
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.86	0.44
1:C:553:GLN:HE21	1:C:556:VAL:HA	1.83	0.44
2:D:198:LEU:HD21	2:D:268:MET:HE3	2.00	0.44
1:A:553:GLN:HE21	1:A:556:VAL:HA	1.83	0.44
1:C:333:MET:HA	1:C:394:GLU:HB2	1.98	0.44
1:A:1160:LEU:O	1:A:1164:SER:OG	2.31	0.44
2:B:74:SER:O	2:B:102:GLN:HB3	2.18	0.43
1:A:158:SER:HB3	2:D:149:GLY:O	2.18	0.43
1:C:1030:THR:N	1:C:1032:GLN:OE1	2.52	0.43
2:B:149:GLY:O	1:C:158:SER:HB3	2.18	0.43
1:C:408:TRP:CD2	1:C:409:PRO:HD2	2.54	0.43
1:A:408:TRP:CD2	1:A:409:PRO:HD2	2.54	0.43
2:D:74:SER:O	2:D:102:GLN:HB3	2.19	0.43
1:A:69:GLU:N	1:A:70:PRO:HD2	2.34	0.43
1:A:1030:THR:N	1:A:1032:GLN:OE1	2.52	0.43
1:A:1090:ALA:HB2	1:A:1144:HIS:CE1	2.54	0.43
1:A:340:MET:HB2	1:A:349:GLY:HA2	2.01	0.42
1:A:571:LEU:HD12	1:A:571:LEU:HA	1.91	0.42
1:C:1131:ARG:HD2	5:C:1604:HEC:HMB2	2.01	0.42
1:A:199:SER:OG	1:A:200:GLY:N	2.53	0.42
1:C:1090:ALA:HB2	1:C:1144:HIS:CE1	2.54	0.42
1:A:172:TRP:CH2	1:A:316:PRO:HG3	2.55	0.42
1:A:1131:ARG:HD2	5:A:1604:HEC:HMB2	2.01	0.42
1:C:199:SER:OG	1:C:200:GLY:N	2.53	0.42
1:C:340:MET:HB2	1:C:349:GLY:HA2	2.01	0.42
1:A:93:ARG:HD2	1:A:301:LYS:HE3	2.01	0.42
1:C:403:ASP:N	1:C:403:ASP:OD1	2.52	0.42
1:A:403:ASP:N	1:A:403:ASP:OD1	2.52	0.42
1:C:69:GLU:N	1:C:70:PRO:HD2	2.34	0.42
2:B:123:THR:O	3:E:5:MAN:O3	2.26	0.42
1:C:172:TRP:CH2	1:C:316:PRO:HG3	2.55	0.42
1:C:1160:LEU:O	1:C:1164:SER:OG	2.31	0.42
1:C:39:LEU:HA	2:D:90:PHE:CZ	2.55	0.41
1:C:1066:TYR:CZ	1:C:1087:ARG:HD3	2.55	0.41
2:D:46:ARG:O	2:D:50:ARG:HG3	2.21	0.41
1:A:1066:TYR:CZ	1:A:1087:ARG:HD3	2.55	0.41
2:B:46:ARG:O	2:B:50:ARG:HG3	2.21	0.41
1:C:93:ARG:HD2	1:C:301:LYS:HE3	2.01	0.41
1:C:541:LEU:O	1:C:545:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:TYR:OH	2:B:158:ALA:O	2.32	0.41
1:A:105:HIS:O	1:A:108:SER:OG	2.29	0.40
1:A:541:LEU:O	1:A:545:THR:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	828/1536 (54%)	788 (95%)	40 (5%)	0	100	100
1	C	828/1536 (54%)	788 (95%)	40 (5%)	0	100	100
2	B	271/341 (80%)	258 (95%)	13 (5%)	0	100	100
2	D	271/341 (80%)	258 (95%)	13 (5%)	0	100	100
All	All	2198/3754 (59%)	2092 (95%)	106 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	702/1348 (52%)	694 (99%)	8 (1%)	73	90
1	C	702/1348 (52%)	694 (99%)	8 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	219/287 (76%)	215 (98%)	4 (2%)	59 83
2	D	219/287 (76%)	215 (98%)	4 (2%)	59 83
All	All	1842/3270 (56%)	1818 (99%)	24 (1%)	70 87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	64	TYR
1	A	244	PHE
1	A	272	ASP
1	A	296	LEU
1	A	468	THR
1	A	480	GLU
1	A	1189	THR
2	B	70	VAL
2	B	115	THR
2	B	162	THR
2	B	240	THR
1	C	23	ASN
1	C	64	TYR
1	C	244	PHE
1	C	272	ASP
1	C	296	LEU
1	C	468	THR
1	C	480	GLU
1	C	1189	THR
2	D	70	VAL
2	D	115	THR
2	D	162	THR
2	D	240	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	105	HIS
1	A	165	GLN
1	A	210	GLN
1	A	225	GLN

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Mol	Chain	Res	Type
1	A	240	ASN
1	A	246	GLN
1	A	289	ASN
1	A	302	GLN
1	A	328	GLN
1	A	376	GLN
1	A	391	GLN
1	A	504	GLN
1	A	1144	HIS
1	A	1188	GLN
1	A	1212	HIS
2	B	82	ASN
2	B	119	GLN
2	B	171	ASN
2	B	195	ASN
2	B	208	HIS
1	C	23	ASN
1	C	105	HIS
1	C	165	GLN
1	C	210	GLN
1	C	225	GLN
1	C	240	ASN
1	C	246	GLN
1	C	289	ASN
1	C	302	GLN
1	C	328	GLN
1	C	376	GLN
1	C	391	GLN
1	C	504	GLN
1	C	1144	HIS
1	C	1188	GLN
1	C	1212	HIS
2	D	82	ASN
2	D	119	GLN
2	D	171	ASN
2	D	195	ASN
2	D	208	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

22 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	0.39	0	17,19,21	0.55	0
3	MAN	E	10	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
3	MAN	E	11	3	11,11,12	0.69	0	15,15,17	1.14	2 (13%)
3	NAG	E	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.89	0
3	BMA	E	3	3	11,11,12	0.66	0	15,15,17	0.81	1 (6%)
3	MAN	E	4	3	11,11,12	0.82	0	15,15,17	1.25	2 (13%)
3	MAN	E	5	3	11,11,12	0.91	0	15,15,17	1.38	2 (13%)
3	MAN	E	6	3	11,11,12	0.90	1 (9%)	15,15,17	0.95	1 (6%)
3	MAN	E	7	3	11,11,12	0.79	0	15,15,17	1.16	2 (13%)
3	MAN	E	8	3	11,11,12	0.70	0	15,15,17	1.22	2 (13%)
3	MAN	E	9	3	11,11,12	0.82	1 (9%)	15,15,17	0.86	1 (6%)
3	NAG	F	1	3,2	14,14,15	0.39	0	17,19,21	0.55	0
3	MAN	F	10	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
3	MAN	F	11	3	11,11,12	0.69	0	15,15,17	1.13	2 (13%)
3	NAG	F	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.88	0
3	BMA	F	3	3	11,11,12	0.66	0	15,15,17	0.81	1 (6%)
3	MAN	F	4	3	11,11,12	0.81	0	15,15,17	1.25	2 (13%)
3	MAN	F	5	3	11,11,12	0.91	0	15,15,17	1.38	2 (13%)
3	MAN	F	6	3	11,11,12	0.90	1 (9%)	15,15,17	0.95	1 (6%)
3	MAN	F	7	3	11,11,12	0.78	0	15,15,17	1.16	2 (13%)
3	MAN	F	8	3	11,11,12	0.70	0	15,15,17	1.22	2 (13%)
3	MAN	F	9	3	11,11,12	0.81	1 (9%)	15,15,17	0.86	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	MAN	E	10	3	-	0/2/19/22	0/1/1/1
3	MAN	E	11	3	-	0/2/19/22	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	MAN	E	8	3	-	1/2/19/22	0/1/1/1
3	MAN	E	9	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
3	MAN	F	10	3	-	0/2/19/22	0/1/1/1
3	MAN	F	11	3	-	0/2/19/22	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	2/2/19/22	0/1/1/1
3	MAN	F	8	3	-	1/2/19/22	0/1/1/1
3	MAN	F	9	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	-2.52	1.39	1.43
3	F	2	NAG	O5-C1	-2.52	1.39	1.43
3	E	9	MAN	O5-C1	-2.52	1.39	1.43
3	F	9	MAN	O5-C1	-2.51	1.39	1.43
3	E	6	MAN	O5-C1	-2.38	1.39	1.43
3	F	6	MAN	O5-C1	-2.37	1.39	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	5	MAN	C1-O5-C5	3.73	117.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	5	MAN	C1-O5-C5	3.71	117.21	112.19
3	E	5	MAN	O2-C2-C3	-3.19	103.75	110.14
3	F	5	MAN	O2-C2-C3	-3.18	103.77	110.14
3	E	8	MAN	O2-C2-C3	-3.17	103.79	110.14
3	F	8	MAN	O2-C2-C3	-3.16	103.82	110.14
3	F	4	MAN	C1-O5-C5	2.99	116.24	112.19
3	F	4	MAN	O2-C2-C3	-2.98	104.16	110.14
3	E	4	MAN	C1-O5-C5	2.97	116.22	112.19
3	E	4	MAN	O2-C2-C3	-2.97	104.19	110.14
3	E	10	MAN	O2-C2-C3	-2.90	104.33	110.14
3	F	10	MAN	O2-C2-C3	-2.89	104.34	110.14
3	E	11	MAN	C1-O5-C5	2.89	116.10	112.19
3	F	7	MAN	O2-C2-C3	-2.85	104.43	110.14
3	E	7	MAN	O2-C2-C3	-2.85	104.43	110.14
3	F	11	MAN	C1-O5-C5	2.84	116.05	112.19
3	F	8	MAN	C1-O5-C5	2.70	115.85	112.19
3	E	8	MAN	C1-O5-C5	2.69	115.83	112.19
3	F	6	MAN	O2-C2-C3	-2.61	104.90	110.14
3	E	6	MAN	O2-C2-C3	-2.60	104.94	110.14
3	F	11	MAN	O2-C2-C3	-2.41	105.30	110.14
3	E	11	MAN	O2-C2-C3	-2.41	105.31	110.14
3	E	7	MAN	C1-O5-C5	2.32	115.33	112.19
3	F	7	MAN	C1-O5-C5	2.31	115.32	112.19
3	F	9	MAN	O2-C2-C3	-2.28	105.57	110.14
3	E	9	MAN	O2-C2-C3	-2.28	105.57	110.14
3	E	3	BMA	O2-C2-C3	-2.14	105.85	110.14
3	F	10	MAN	C1-O5-C5	2.13	115.08	112.19
3	F	3	BMA	O2-C2-C3	-2.13	105.87	110.14
3	E	10	MAN	C1-O5-C5	2.13	115.07	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	7	MAN	C4-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	E	7	MAN	O5-C5-C6-O6
3	F	7	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	4	MAN	C4-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	E	8	MAN	O5-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6

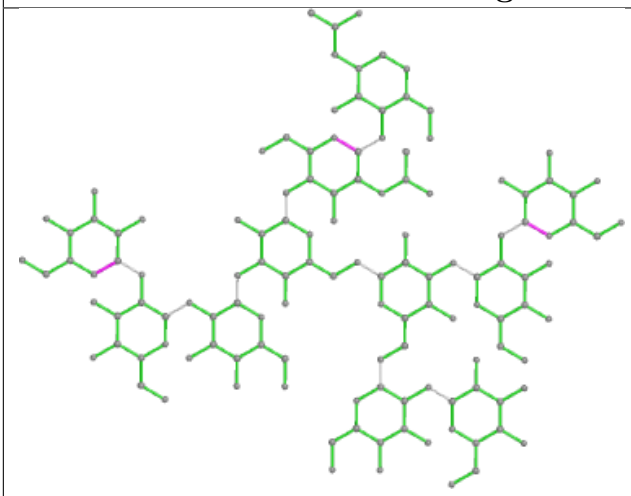
There are no ring outliers.

4 monomers are involved in 4 short contacts:

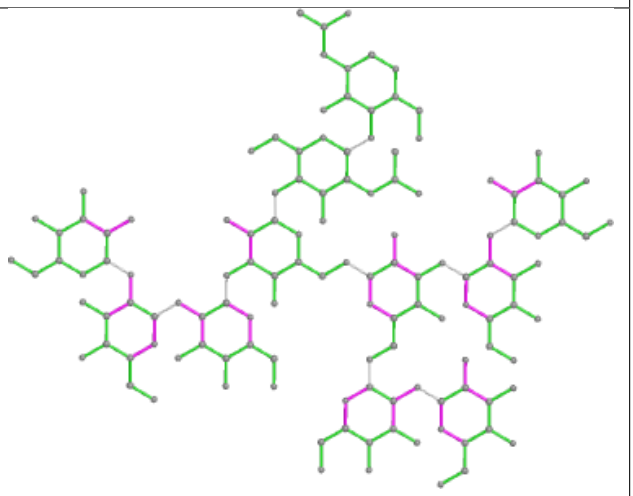
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	E	5	MAN	1	0
3	F	5	MAN	1	0
3	F	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

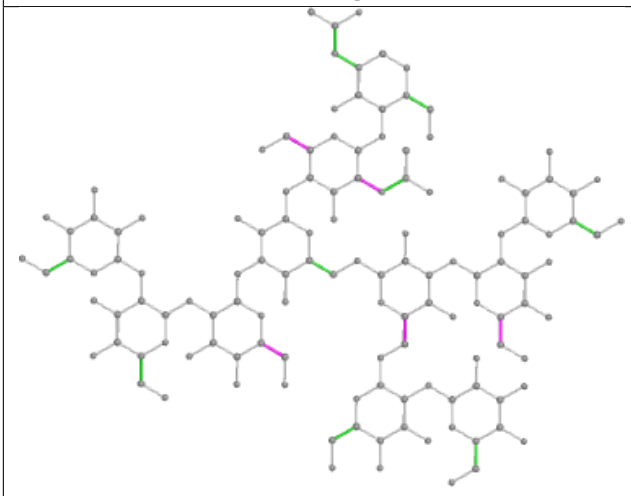
Oligosaccharide Chain E



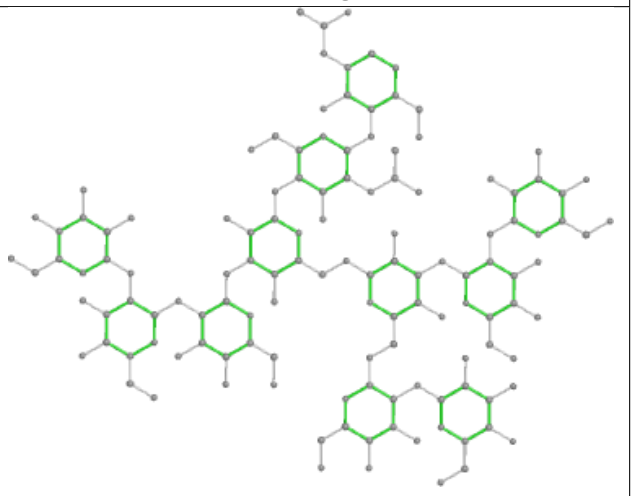
Bond lengths



Bond angles

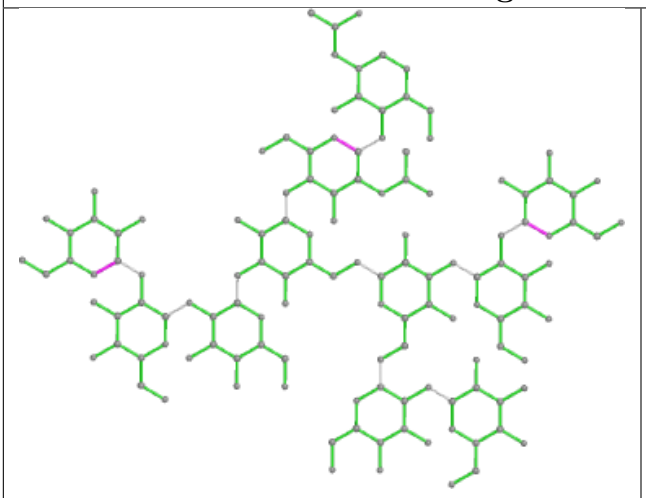


Torsions

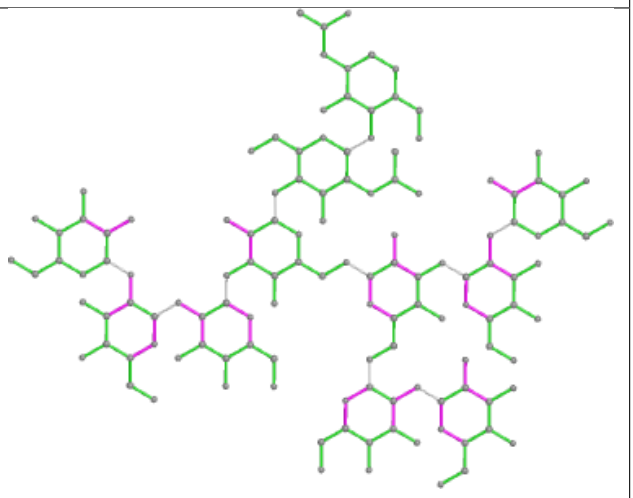


Rings

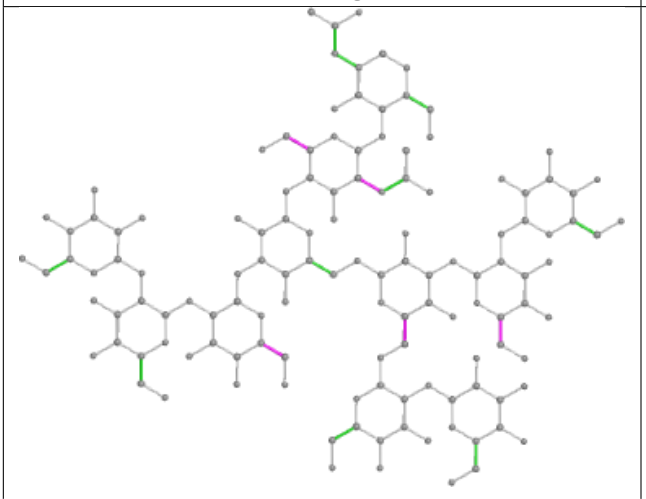
Oligosaccharide Chain F



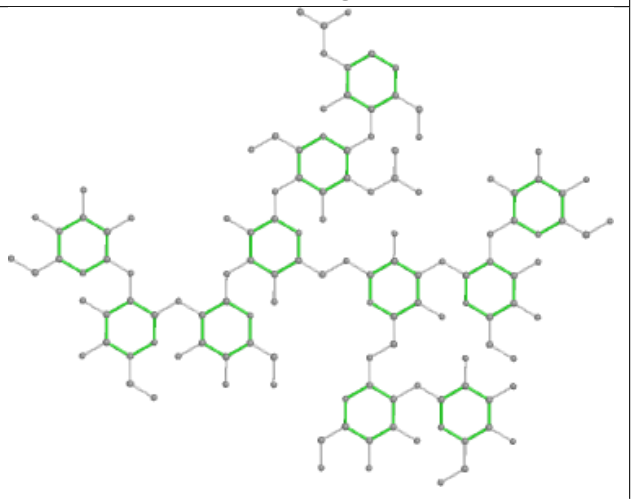
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	401	2	14,14,15	0.20	0	17,19,21	0.48	0
5	HEC	C	1605	1	32,50,50	1.71	8 (25%)	24,82,82	1.63	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	413	2	14,14,15	0.23	0	17,19,21	0.38	0
6	PX2	A	1606	-	35,35,35	1.08	2 (5%)	39,40,40	1.38	5 (12%)
4	NAG	A	1601	1	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	D	401	2	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	A	1602	1	14,14,15	0.38	0	17,19,21	0.33	0
5	HEC	A	1604	1	32,50,50	1.72	8 (25%)	24,82,82	1.59	5 (20%)
6	PX2	C	1606	-	35,35,35	1.08	2 (5%)	39,40,40	1.38	5 (12%)
7	PLC	B	414	-	41,41,41	1.01	3 (7%)	47,49,49	1.35	4 (8%)
4	NAG	C	1601	1	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	C	1602	1	14,14,15	0.38	0	17,19,21	0.33	0
4	NAG	A	1603	1	14,14,15	0.56	0	17,19,21	1.29	1 (5%)
4	NAG	C	1603	1	14,14,15	0.58	0	17,19,21	1.29	1 (5%)
4	NAG	D	413	2	14,14,15	0.23	0	17,19,21	0.38	0
5	HEC	A	1605	1	32,50,50	1.71	8 (25%)	24,82,82	1.64	6 (25%)
7	PLC	D	414	-	41,41,41	1.01	3 (7%)	47,49,49	1.35	4 (8%)
5	HEC	C	1604	1	32,50,50	1.72	8 (25%)	24,82,82	1.59	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	401	2	-	2/6/23/26	0/1/1/1
5	HEC	C	1605	1	-	2/10/54/54	-
4	NAG	B	413	2	-	2/6/23/26	0/1/1/1
6	PX2	A	1606	-	-	18/37/37/37	-
4	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
4	NAG	D	401	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1602	1	-	2/6/23/26	0/1/1/1
5	HEC	A	1604	1	-	4/10/54/54	-
6	PX2	C	1606	-	-	18/37/37/37	-
7	PLC	B	414	-	-	20/45/45/45	-
4	NAG	C	1601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1602	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1603	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1603	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	413	2	-	2/6/23/26	0/1/1/1
5	HEC	A	1605	1	-	2/10/54/54	-
7	PLC	D	414	-	-	20/45/45/45	-
5	HEC	C	1604	1	-	4/10/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1604	HEC	CBC-CAC	-4.86	1.31	1.49
5	A	1604	HEC	CBC-CAC	-4.85	1.31	1.49
5	C	1605	HEC	CBC-CAC	-4.75	1.31	1.49
5	A	1605	HEC	CBC-CAC	-4.73	1.31	1.49
5	A	1604	HEC	CBB-CAB	-4.73	1.31	1.49
5	C	1604	HEC	CBB-CAB	-4.73	1.31	1.49
5	A	1605	HEC	CBB-CAB	-4.63	1.32	1.49
5	C	1605	HEC	CBB-CAB	-4.62	1.32	1.49
6	A	1606	PX2	O7-C16	4.02	1.45	1.34
6	C	1606	PX2	O7-C16	4.02	1.45	1.34
6	A	1606	PX2	O5-C4	3.61	1.43	1.33
6	C	1606	PX2	O5-C4	3.58	1.43	1.33
7	B	414	PLC	O3-CB	3.41	1.43	1.33
7	D	414	PLC	O3-CB	3.39	1.43	1.33
7	D	414	PLC	O2-C'	3.34	1.43	1.34
7	B	414	PLC	O2-C'	3.34	1.43	1.34
5	C	1604	HEC	C3C-C4C	-3.01	1.37	1.43
5	A	1604	HEC	C3C-C4C	-3.00	1.37	1.43
5	C	1605	HEC	C3C-C4C	-2.88	1.37	1.43
5	A	1605	HEC	C3C-C4C	-2.86	1.37	1.43
5	A	1604	HEC	C4B-C3B	-2.70	1.38	1.43
5	C	1604	HEC	C4B-C3B	-2.66	1.38	1.43
5	A	1605	HEC	C4B-C3B	-2.54	1.38	1.43
5	C	1605	HEC	C4B-C3B	-2.49	1.38	1.43
5	A	1604	HEC	O1A-CGA	2.34	1.29	1.22
5	C	1604	HEC	O1A-CGA	2.34	1.29	1.22
5	A	1604	HEC	O1D-CGD	2.29	1.29	1.22
5	C	1604	HEC	O1D-CGD	2.29	1.29	1.22
5	A	1605	HEC	O1A-CGA	2.24	1.29	1.22
5	C	1605	HEC	O1A-CGA	2.24	1.29	1.22
7	D	414	PLC	O3-C3	-2.21	1.40	1.45
5	C	1605	HEC	O1D-CGD	2.21	1.29	1.22
5	A	1605	HEC	O1D-CGD	2.19	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	414	PLC	O3-C3	-2.18	1.40	1.45
5	A	1605	HEC	O2D-CGD	-2.08	1.23	1.30
5	A	1604	HEC	O2D-CGD	-2.07	1.23	1.30
5	C	1604	HEC	O2D-CGD	-2.07	1.23	1.30
5	C	1605	HEC	O2D-CGD	-2.07	1.23	1.30
5	A	1605	HEC	O2A-CGA	-2.06	1.23	1.30
5	C	1605	HEC	O2A-CGA	-2.06	1.23	1.30
5	A	1604	HEC	O2A-CGA	-2.02	1.23	1.30
5	C	1604	HEC	O2A-CGA	-2.02	1.23	1.30

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	414	PLC	O2-C'-C1'	5.67	123.73	111.50
7	D	414	PLC	O2-C'-C1'	5.67	123.72	111.50
4	A	1603	NAG	C2-N2-C7	4.22	128.91	122.90
4	C	1603	NAG	C2-N2-C7	4.22	128.91	122.90
6	A	1606	PX2	C3-C2-C1	-3.75	102.92	111.79
6	C	1606	PX2	C3-C2-C1	-3.73	102.96	111.79
5	C	1605	HEC	CMB-C2B-C3B	3.21	129.59	125.82
5	A	1605	HEC	CMB-C2B-C3B	3.20	129.59	125.82
5	A	1604	HEC	CMB-C2B-C3B	3.18	129.56	125.82
5	C	1604	HEC	CMB-C2B-C3B	3.18	129.56	125.82
7	B	414	PLC	O2-C'-O'	-3.07	116.28	123.70
7	D	414	PLC	O2-C'-O'	-3.07	116.28	123.70
6	A	1606	PX2	O5-C4-C5	2.97	121.23	111.91
6	C	1606	PX2	O5-C4-C5	2.97	121.22	111.91
6	A	1606	PX2	O7-C16-C17	2.90	117.76	111.50
6	C	1606	PX2	O7-C16-C17	2.90	117.76	111.50
5	A	1604	HEC	C4C-C3C-C2C	2.58	109.13	106.35
5	A	1605	HEC	CMC-C2C-C3C	2.57	128.84	125.82
5	C	1604	HEC	C4C-C3C-C2C	2.55	109.10	106.35
5	C	1605	HEC	CMC-C2C-C3C	2.54	128.81	125.82
5	A	1604	HEC	C2B-C3B-C4B	2.52	109.08	106.35
5	C	1604	HEC	C2B-C3B-C4B	2.52	109.07	106.35
6	A	1606	PX2	O1-P1-O2	2.49	120.44	110.68
6	C	1606	PX2	O1-P1-O2	2.48	120.41	110.68
7	D	414	PLC	O3-CB-C1B	2.48	119.68	111.91
7	B	414	PLC	O3-CB-C1B	2.46	119.63	111.91
5	A	1605	HEC	C2B-C3B-C4B	2.43	108.98	106.35
5	C	1605	HEC	C2B-C3B-C4B	2.41	108.95	106.35
5	A	1605	HEC	C4C-C3C-C2C	2.35	108.89	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	414	PLC	O3-CB-OB	-2.32	117.74	123.59
5	C	1605	HEC	C4C-C3C-C2C	2.32	108.85	106.35
7	B	414	PLC	O3-CB-OB	-2.31	117.77	123.59
5	A	1604	HEC	CMC-C2C-C3C	2.29	128.51	125.82
5	C	1604	HEC	CMC-C2C-C3C	2.29	128.51	125.82
6	A	1606	PX2	O5-C4-O6	-2.28	117.84	123.59
6	C	1606	PX2	O5-C4-O6	-2.27	117.85	123.59
5	A	1605	HEC	CBA-CAA-C2A	-2.21	108.87	112.60
5	A	1604	HEC	CAA-CBA-CGA	-2.20	107.59	113.76
5	C	1604	HEC	CAA-CBA-CGA	-2.19	107.61	113.76
5	C	1605	HEC	CBA-CAA-C2A	-2.19	108.91	112.60
5	A	1605	HEC	CBD-CAD-C3D	-2.01	109.19	112.62

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1606	PX2	C1-O4-P1-O1
6	A	1606	PX2	C1-O4-P1-O2
6	A	1606	PX2	C1-O4-P1-O3
6	C	1606	PX2	C1-O4-P1-O1
6	C	1606	PX2	C1-O4-P1-O2
6	C	1606	PX2	C1-O4-P1-O3
7	B	414	PLC	O4P-C4-C5-N
7	B	414	PLC	C4-O4P-P-O1P
7	B	414	PLC	C4-O4P-P-O2P
7	B	414	PLC	C4-O4P-P-O3P
7	D	414	PLC	O4P-C4-C5-N
7	D	414	PLC	C4-O4P-P-O1P
7	D	414	PLC	C4-O4P-P-O2P
7	D	414	PLC	C4-O4P-P-O3P
4	A	1602	NAG	O5-C5-C6-O6
4	C	1602	NAG	O5-C5-C6-O6
4	A	1603	NAG	C4-C5-C6-O6
4	C	1603	NAG	C4-C5-C6-O6
4	B	401	NAG	C4-C5-C6-O6
4	D	401	NAG	C4-C5-C6-O6
4	A	1603	NAG	O5-C5-C6-O6
4	C	1603	NAG	O5-C5-C6-O6
4	C	1602	NAG	C4-C5-C6-O6
4	A	1602	NAG	C4-C5-C6-O6
4	B	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	401	NAG	O5-C5-C6-O6
6	A	1606	PX2	C5-C4-O5-C3
6	C	1606	PX2	C5-C4-O5-C3
4	A	1603	NAG	C8-C7-N2-C2
4	A	1603	NAG	O7-C7-N2-C2
4	C	1603	NAG	C8-C7-N2-C2
4	C	1603	NAG	O7-C7-N2-C2
6	A	1606	PX2	O6-C4-O5-C3
6	C	1606	PX2	O6-C4-O5-C3
7	B	414	PLC	C'-C1'-C2'-C3'
7	D	414	PLC	C'-C1'-C2'-C3'
4	B	413	NAG	O5-C5-C6-O6
4	D	413	NAG	O5-C5-C6-O6
4	A	1601	NAG	O5-C5-C6-O6
4	C	1601	NAG	O5-C5-C6-O6
6	A	1606	PX2	C16-C17-C18-C19
6	C	1606	PX2	C16-C17-C18-C19
6	A	1606	PX2	C17-C18-C19-C20
6	C	1606	PX2	C17-C18-C19-C20
4	B	413	NAG	C4-C5-C6-O6
4	D	413	NAG	C4-C5-C6-O6
7	B	414	PLC	C1'-C2'-C3'-C4'
7	D	414	PLC	C1'-C2'-C3'-C4'
7	B	414	PLC	C6'-C7'-C8'-C9'
7	D	414	PLC	C6'-C7'-C8'-C9'
7	B	414	PLC	C8B-C9B-CAA-CBA
7	D	414	PLC	C8B-C9B-CAA-CBA
7	B	414	PLC	C7'-C8'-C9'-CA'
7	D	414	PLC	C7'-C8'-C9'-CA'
6	A	1606	PX2	C21-C22-C23-C24
6	C	1606	PX2	C21-C22-C23-C24
6	A	1606	PX2	C9-C10-C11-C12
6	C	1606	PX2	C9-C10-C11-C12
7	B	414	PLC	C5'-C6'-C7'-C8'
7	D	414	PLC	C5'-C6'-C7'-C8'
7	B	414	PLC	C3'-C4'-C5'-C6'
7	D	414	PLC	C3'-C4'-C5'-C6'
6	A	1606	PX2	O4-C1-C2-O7
6	C	1606	PX2	O4-C1-C2-O7
7	B	414	PLC	O3P-C1-C2-O2
7	D	414	PLC	O3P-C1-C2-O2
6	A	1606	PX2	O7-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
6	C	1606	PX2	O7-C2-C3-O5
7	B	414	PLC	C2B-C3B-C4B-C5B
7	D	414	PLC	C2B-C3B-C4B-C5B
7	B	414	PLC	CB-C1B-C2B-C3B
7	D	414	PLC	CB-C1B-C2B-C3B
6	A	1606	PX2	C17-C16-O7-C2
6	C	1606	PX2	C17-C16-O7-C2
6	A	1606	PX2	O8-C16-O7-C2
6	C	1606	PX2	O8-C16-O7-C2
7	B	414	PLC	C1-O3P-P-O4P
7	D	414	PLC	C1-O3P-P-O4P
7	B	414	PLC	C4'-C5'-C6'-C7'
7	D	414	PLC	C4'-C5'-C6'-C7'
6	A	1606	PX2	O4-C1-C2-C3
6	C	1606	PX2	O4-C1-C2-C3
7	B	414	PLC	O3P-C1-C2-C3
7	D	414	PLC	O3P-C1-C2-C3
7	B	414	PLC	C6B-C7B-C8B-C9B
7	D	414	PLC	C6B-C7B-C8B-C9B
6	A	1606	PX2	C18-C19-C20-C21
6	C	1606	PX2	C18-C19-C20-C21
6	A	1606	PX2	C5-C6-C7-C8
6	C	1606	PX2	C5-C6-C7-C8
7	B	414	PLC	C4B-C5B-C6B-C7B
7	D	414	PLC	C4B-C5B-C6B-C7B
4	A	1601	NAG	C4-C5-C6-O6
4	A	1603	NAG	C3-C2-N2-C7
4	C	1603	NAG	C3-C2-N2-C7
4	C	1601	NAG	C4-C5-C6-O6
5	A	1604	HEC	CAA-CBA-CGA-O2A
5	C	1604	HEC	CAA-CBA-CGA-O2A
5	A	1605	HEC	CAA-CBA-CGA-O1A
5	C	1605	HEC	CAA-CBA-CGA-O1A
5	A	1604	HEC	CAA-CBA-CGA-O1A
5	C	1604	HEC	CAA-CBA-CGA-O1A
5	A	1604	HEC	CAD-CBD-CGD-O1D
5	C	1604	HEC	CAD-CBD-CGD-O1D
5	A	1604	HEC	CAD-CBD-CGD-O2D
5	C	1604	HEC	CAD-CBD-CGD-O2D
5	A	1605	HEC	CAA-CBA-CGA-O2A
5	C	1605	HEC	CAA-CBA-CGA-O2A
6	A	1606	PX2	C1-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
6	C	1606	PX2	C1-C2-C3-O5
7	B	414	PLC	C1-O3P-P-O2P
7	D	414	PLC	C1-O3P-P-O2P
6	A	1606	PX2	C12-C13-C14-C15
6	C	1606	PX2	C12-C13-C14-C15

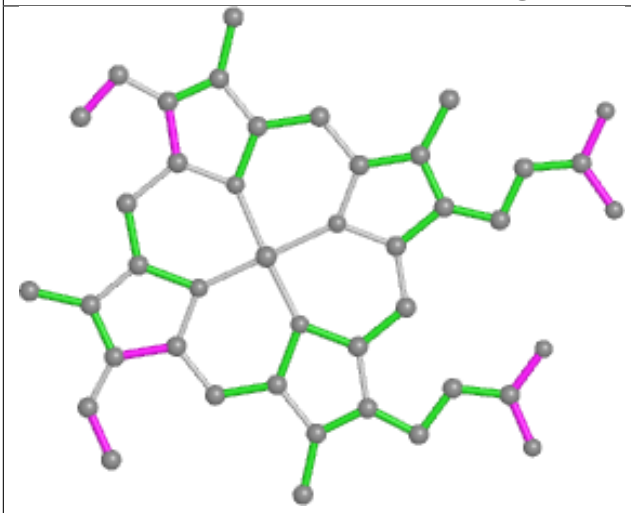
There are no ring outliers.

12 monomers are involved in 24 short contacts:

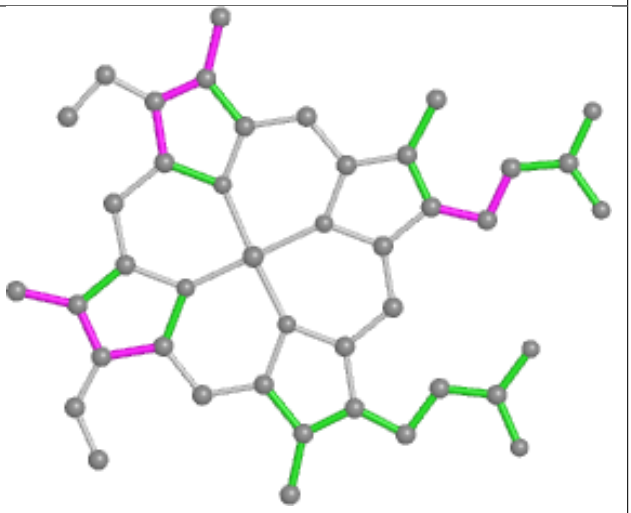
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	NAG	1	0
5	C	1605	HEC	2	0
6	A	1606	PX2	1	0
4	D	401	NAG	1	0
5	A	1604	HEC	5	0
6	C	1606	PX2	1	0
7	B	414	PLC	2	0
4	A	1603	NAG	1	0
4	C	1603	NAG	1	0
5	A	1605	HEC	2	0
7	D	414	PLC	2	0
5	C	1604	HEC	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

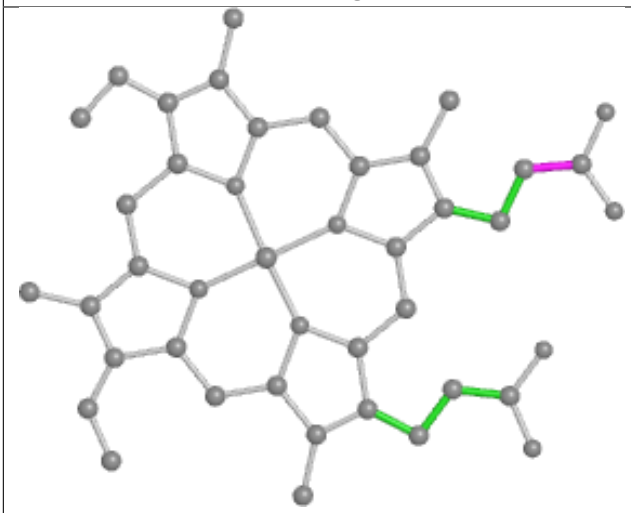
Ligand HEC C 1605



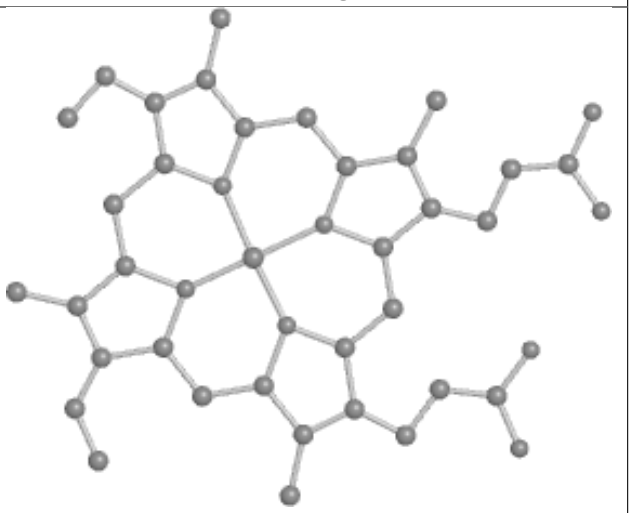
Bond lengths



Bond angles

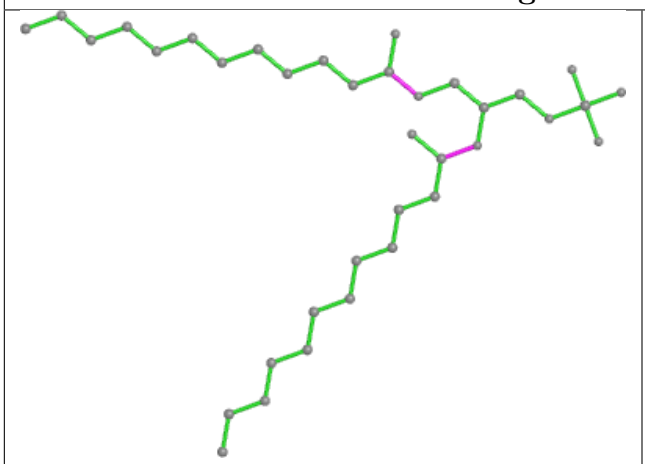


Torsions

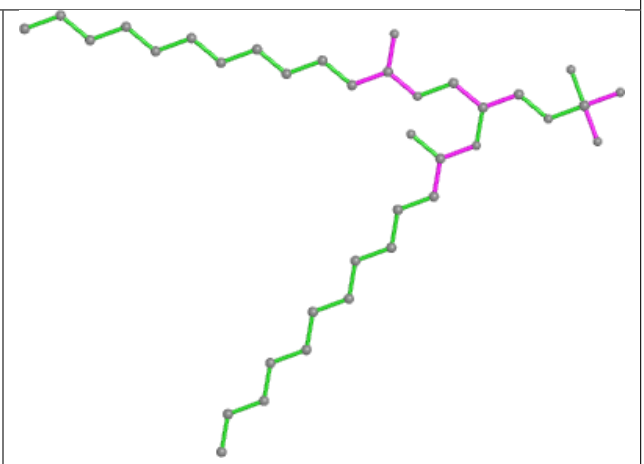


Rings

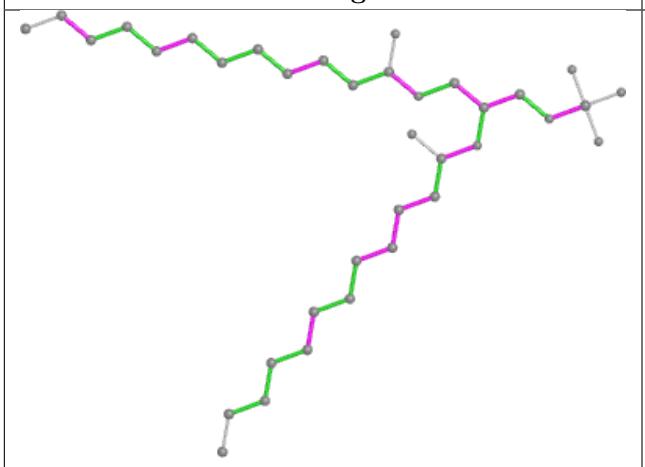
Ligand PX2 A 1606



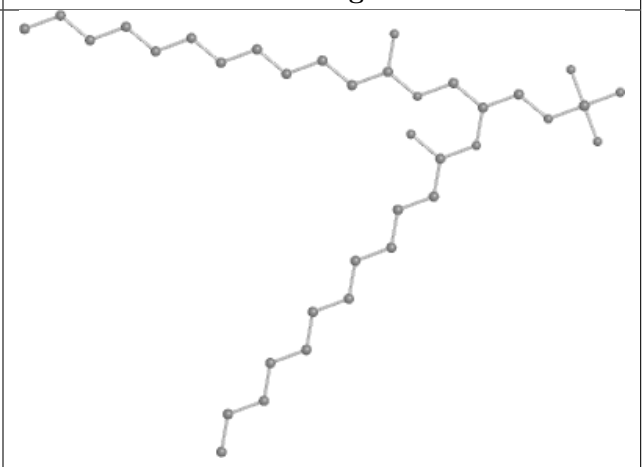
Bond lengths



Bond angles

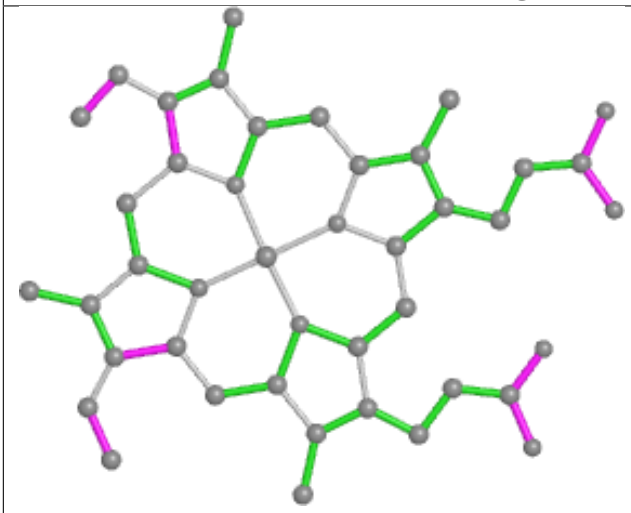


Torsions

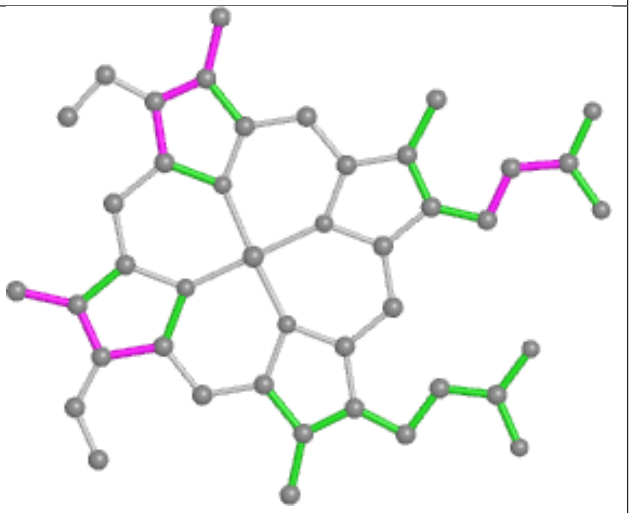


Rings

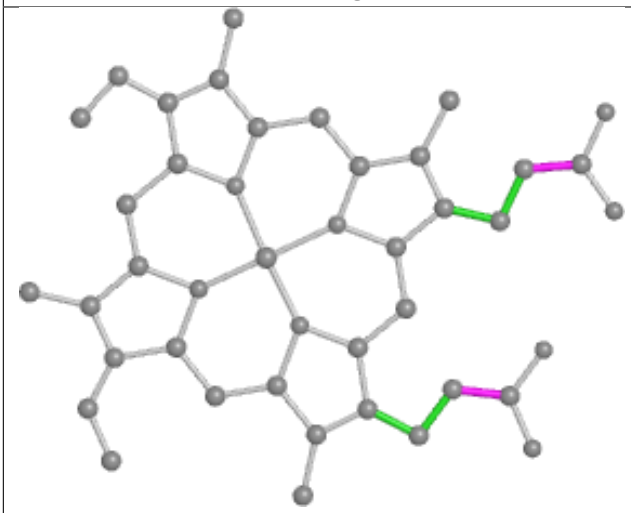
Ligand HEC A 1604



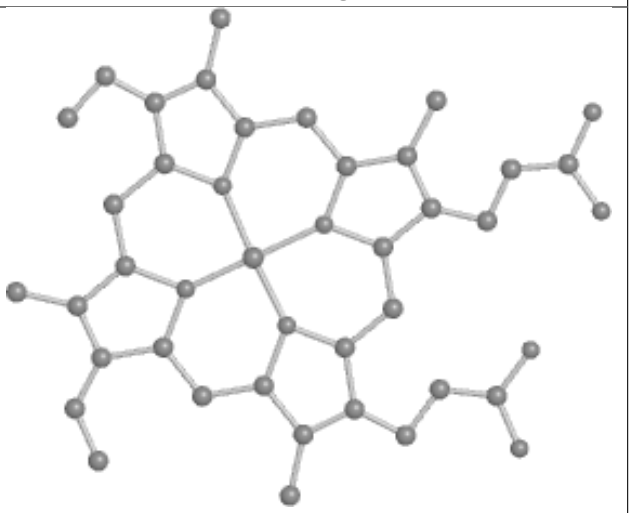
Bond lengths



Bond angles

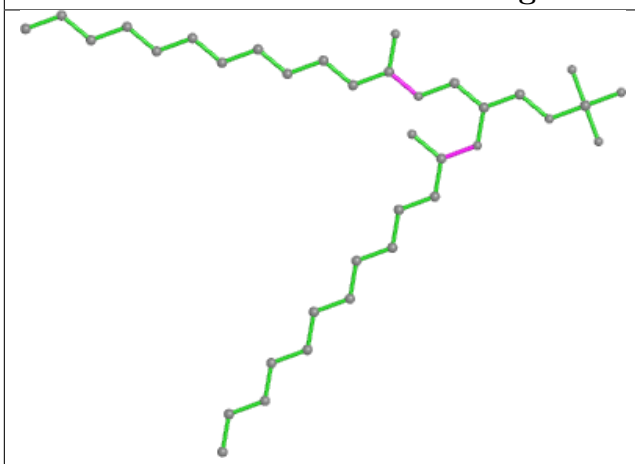


Torsions

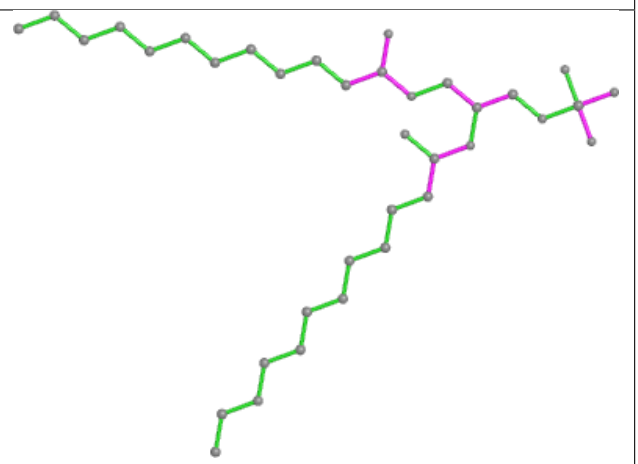


Rings

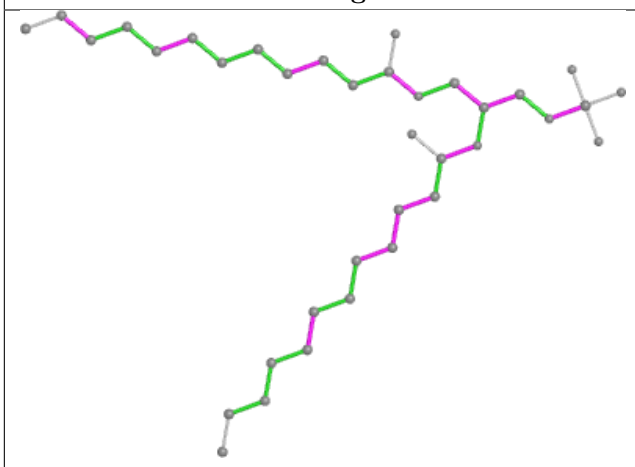
Ligand PX2 C 1606



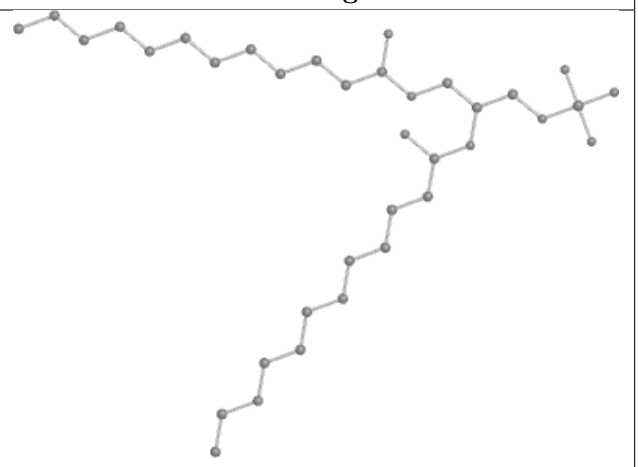
Bond lengths



Bond angles

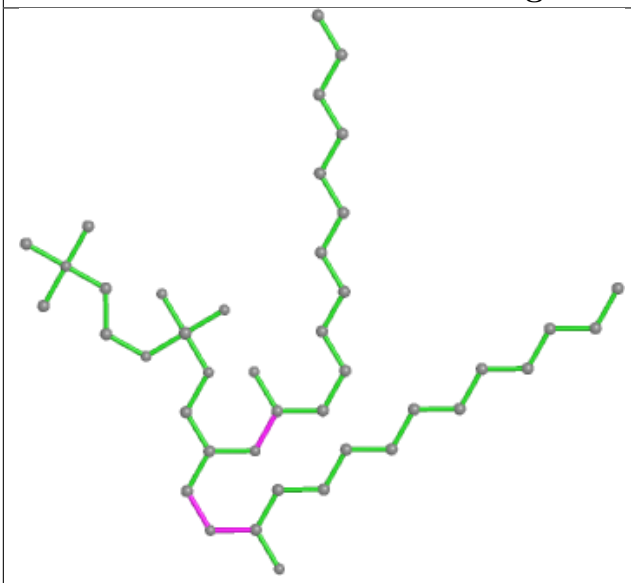


Torsions

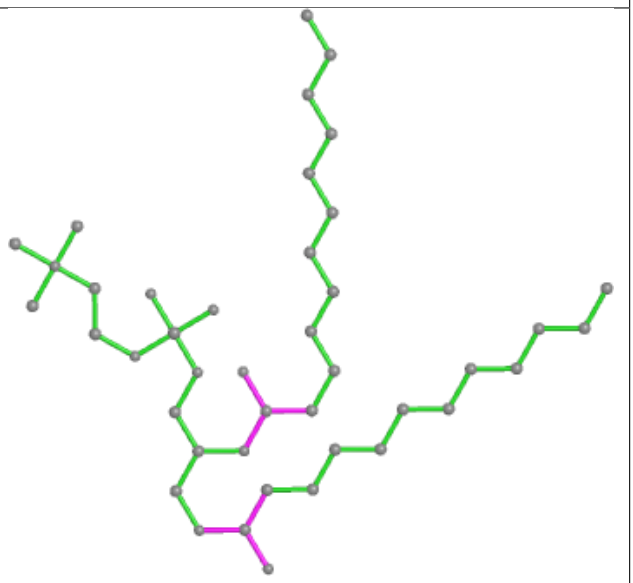


Rings

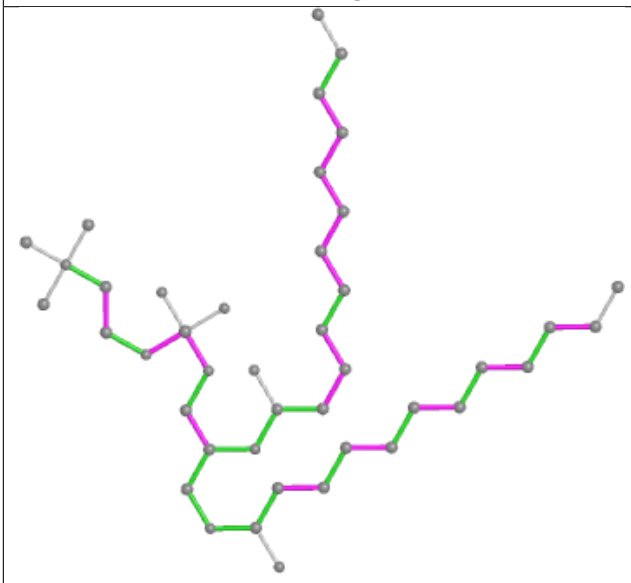
Ligand PLC B 414



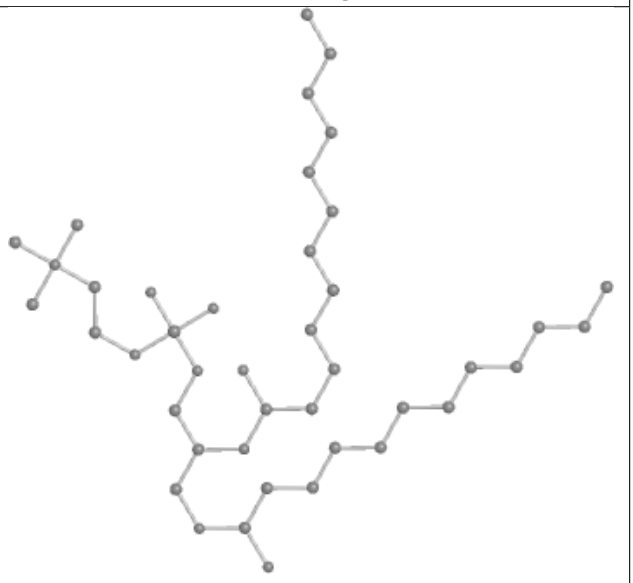
Bond lengths



Bond angles

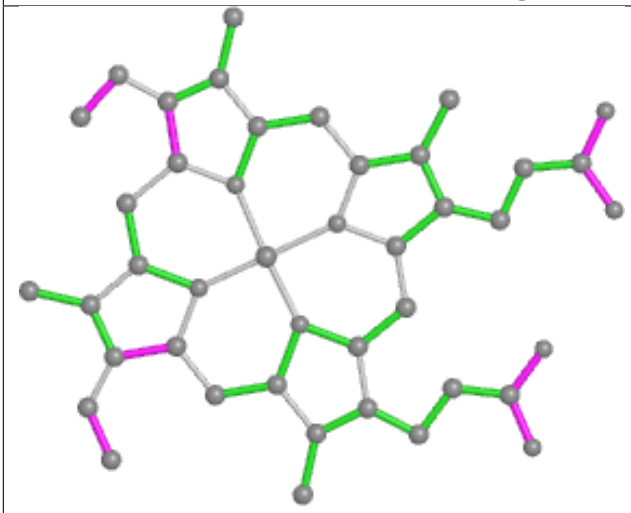


Torsions

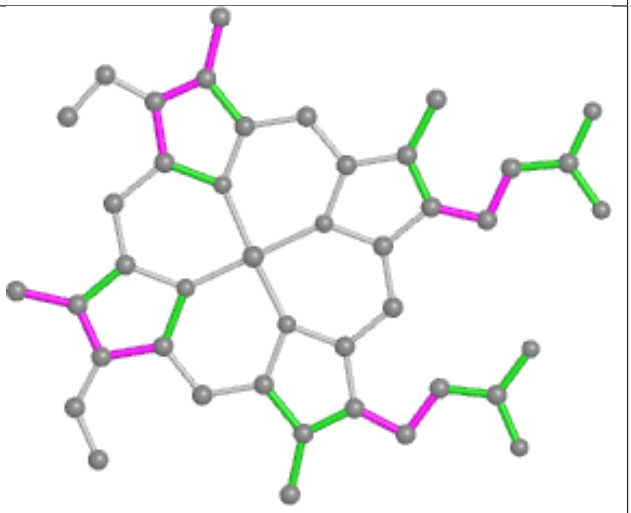


Rings

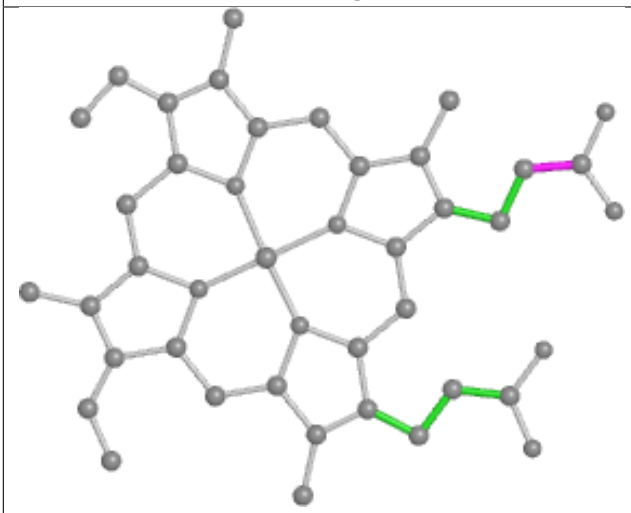
Ligand HEC A 1605



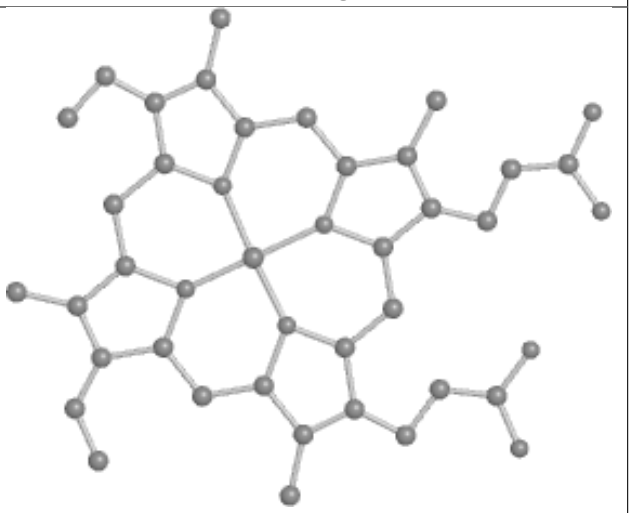
Bond lengths



Bond angles

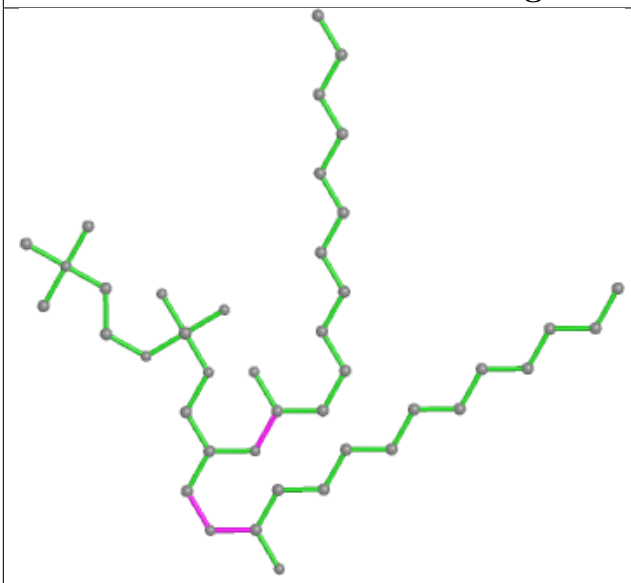


Torsions

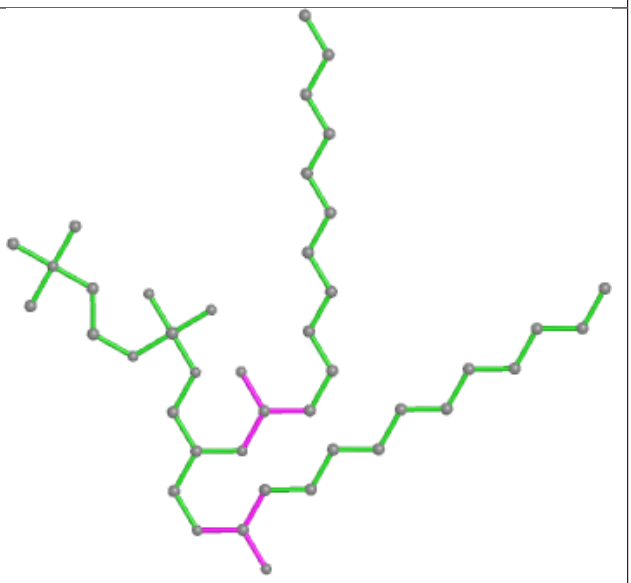


Rings

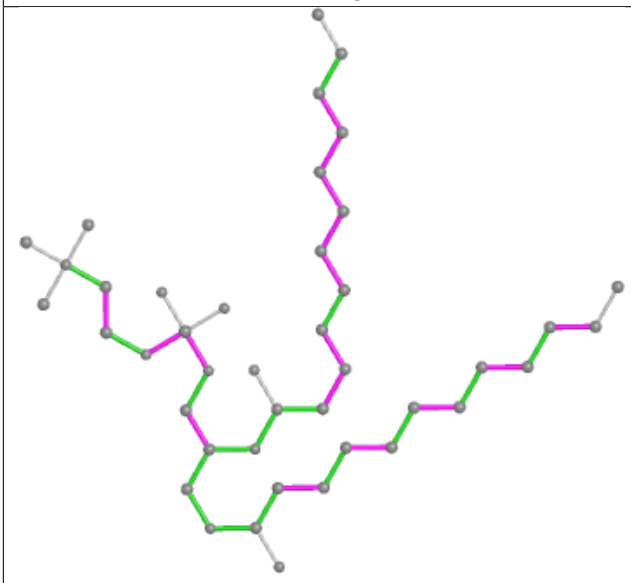
Ligand PLC D 414



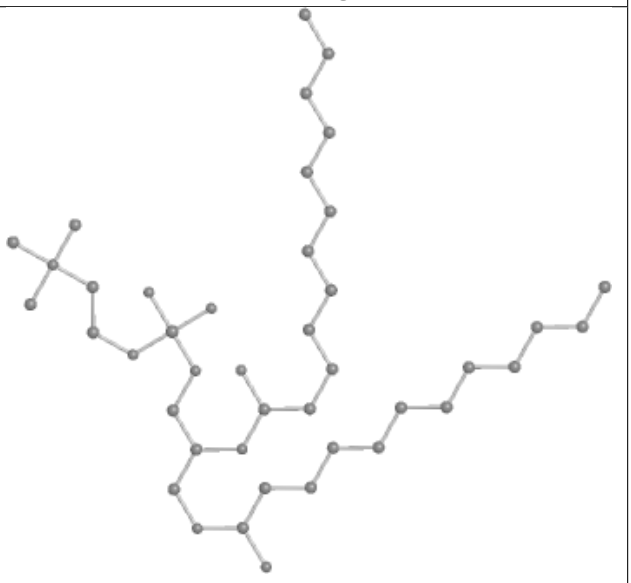
Bond lengths



Bond angles

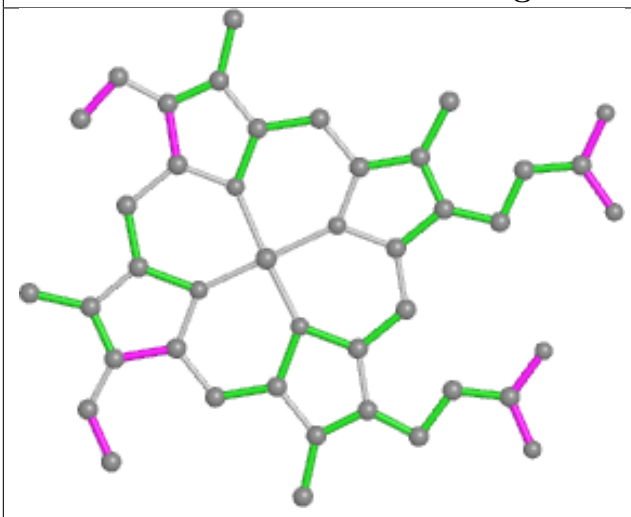


Torsions

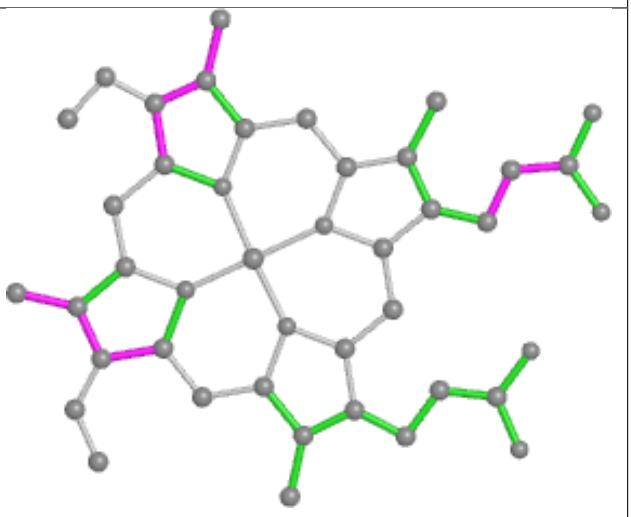


Rings

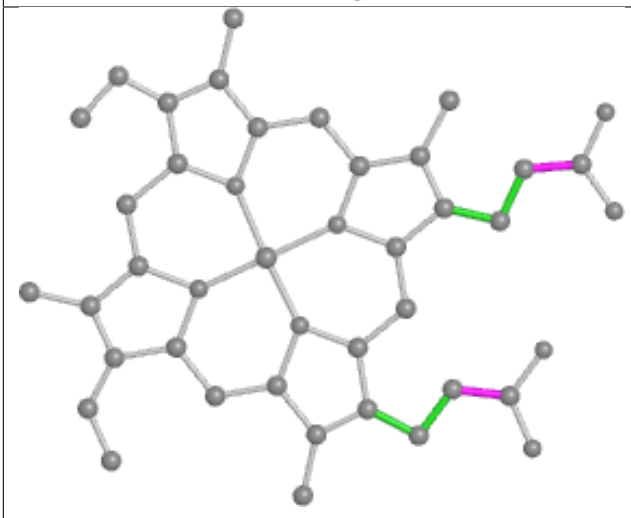
Ligand HEC C 1604



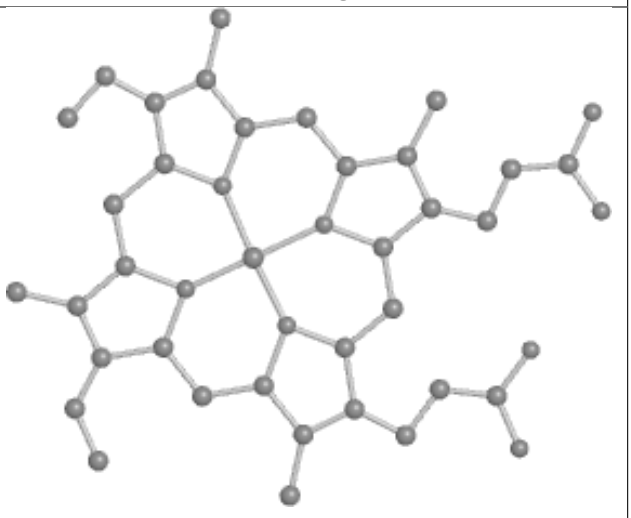
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

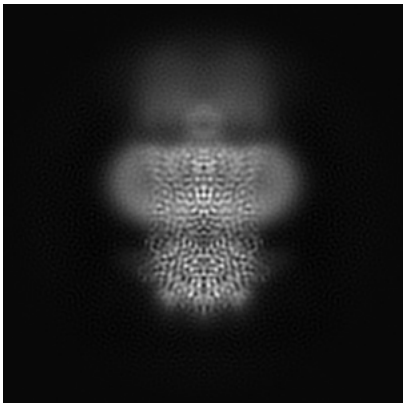
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21963. These allow visual inspection of the internal detail of the map and identification of artifacts.

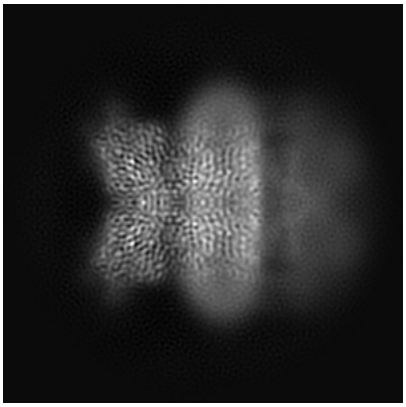
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

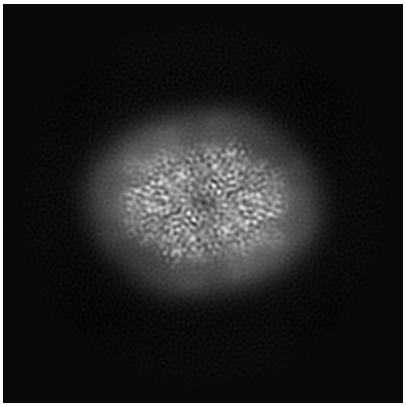
6.1.1 Primary map



X



Y

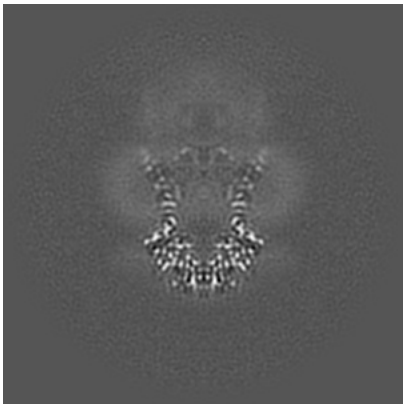


Z

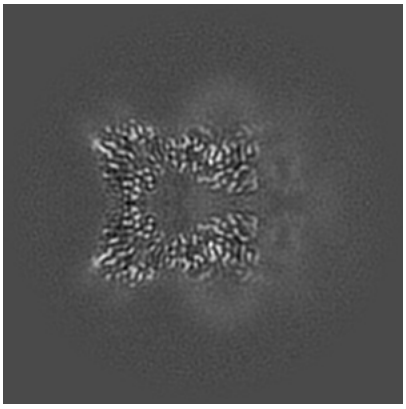
The images above show the map projected in three orthogonal directions.

6.2 Central slices

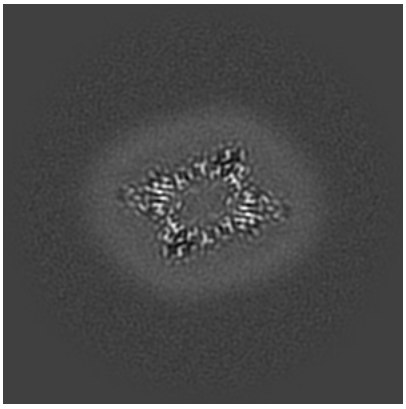
6.2.1 Primary map



X Index: 115



Y Index: 115

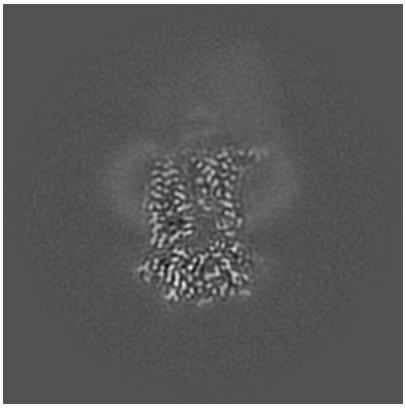


Z Index: 115

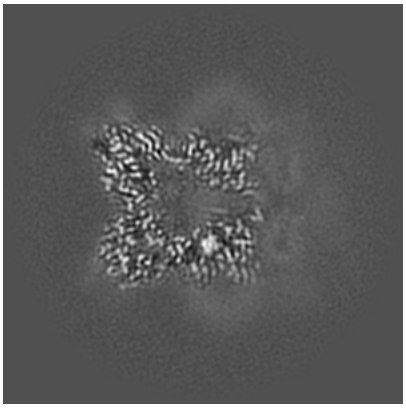
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

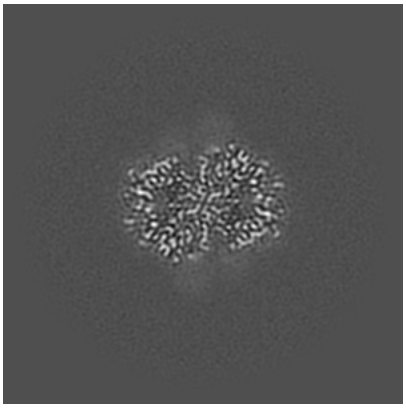
6.3.1 Primary map



X Index: 100



Y Index: 118

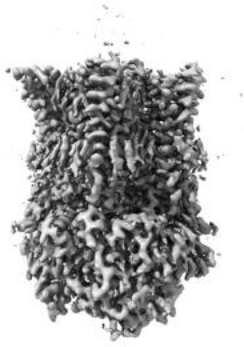


Z Index: 80

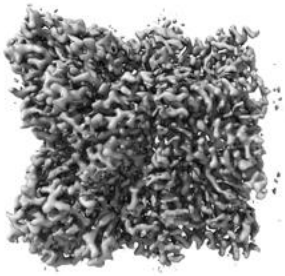
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

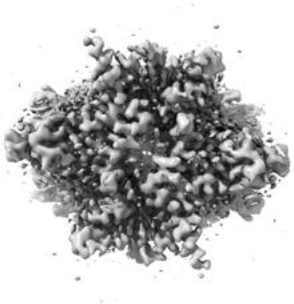
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

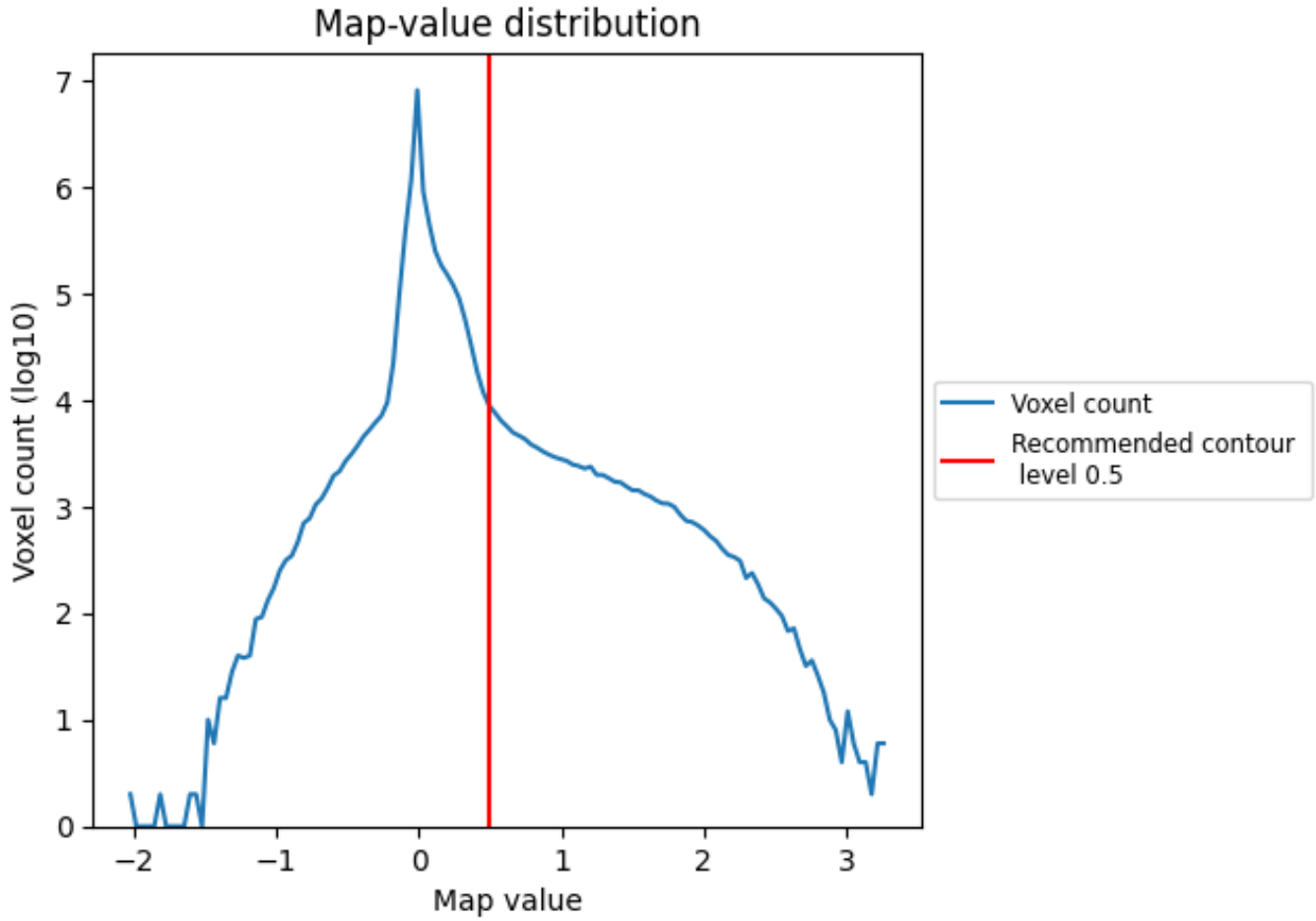
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

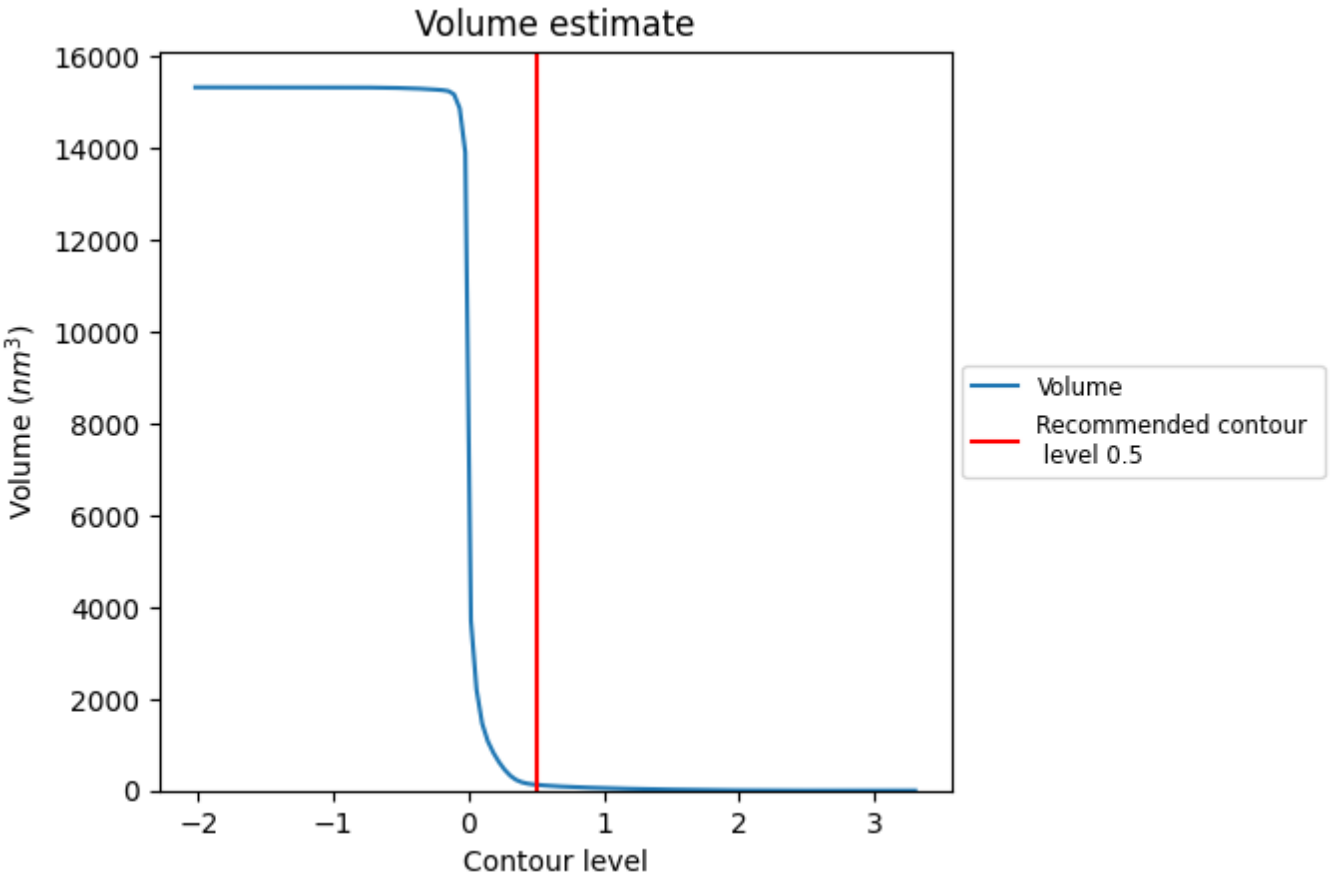
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

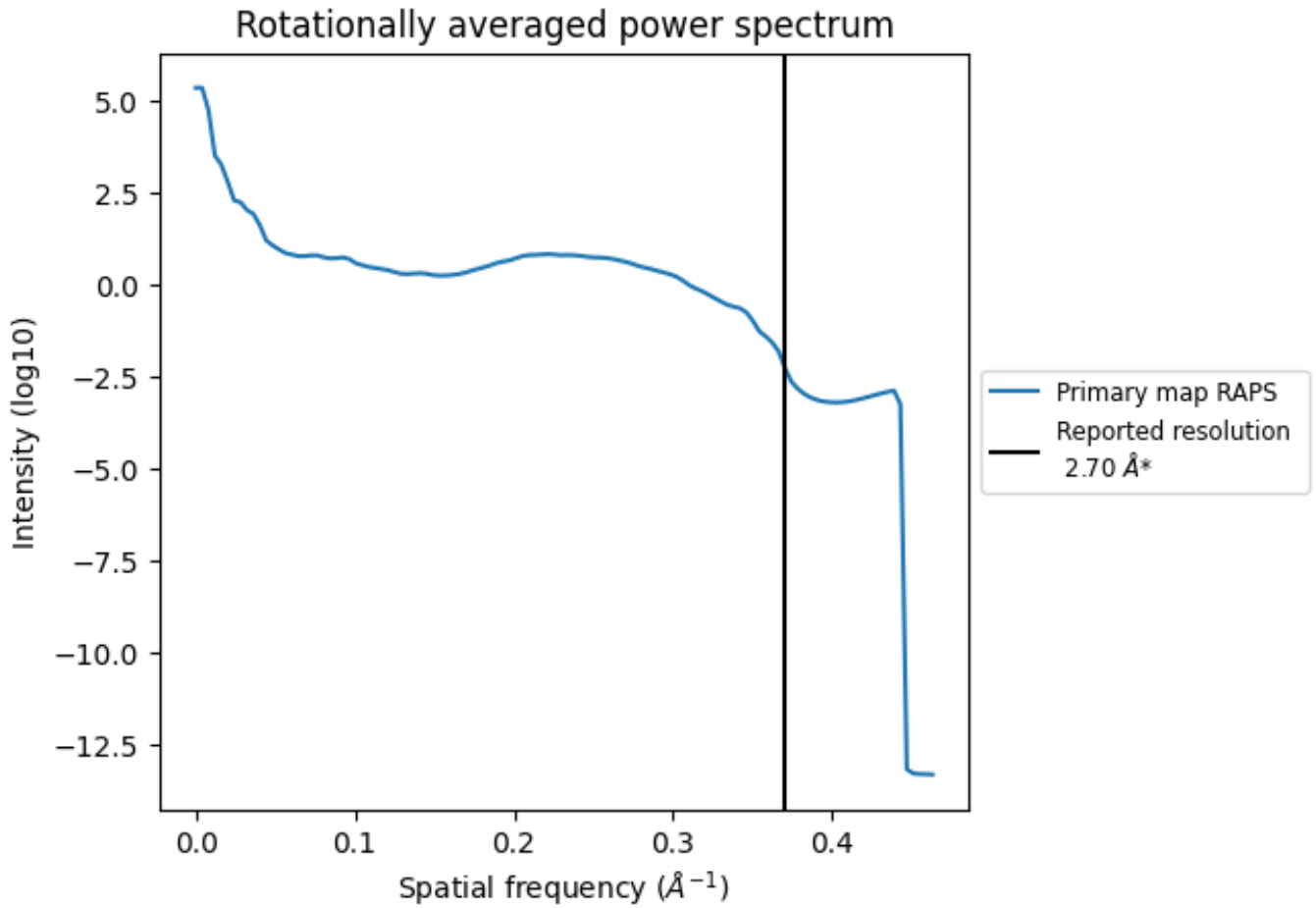
7.2 Volume estimate



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

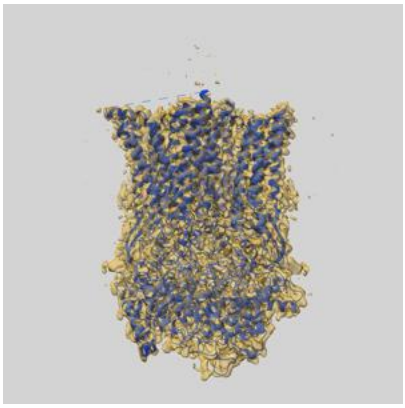
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

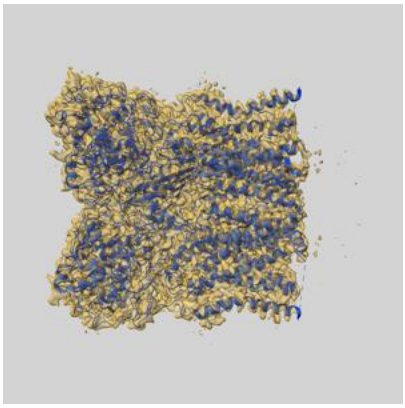
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21963 and PDB model 6WXU. Per-residue inclusion information can be found in section 3 on page 8.

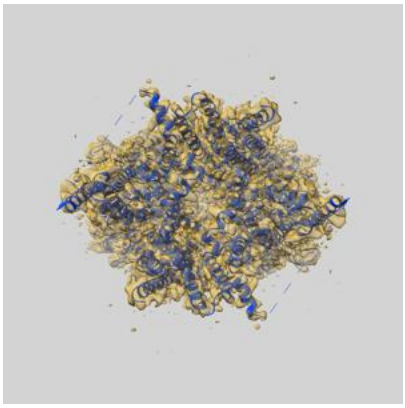
9.1 Map-model overlay



X



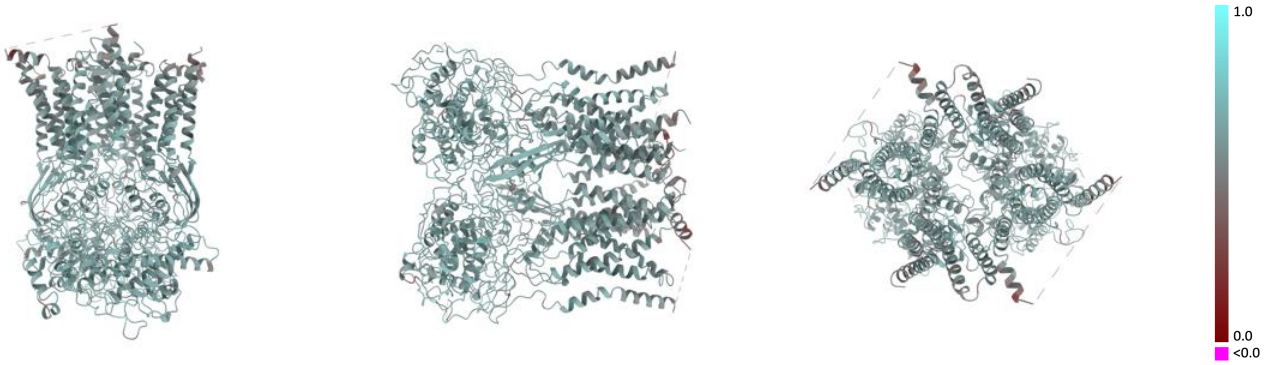
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

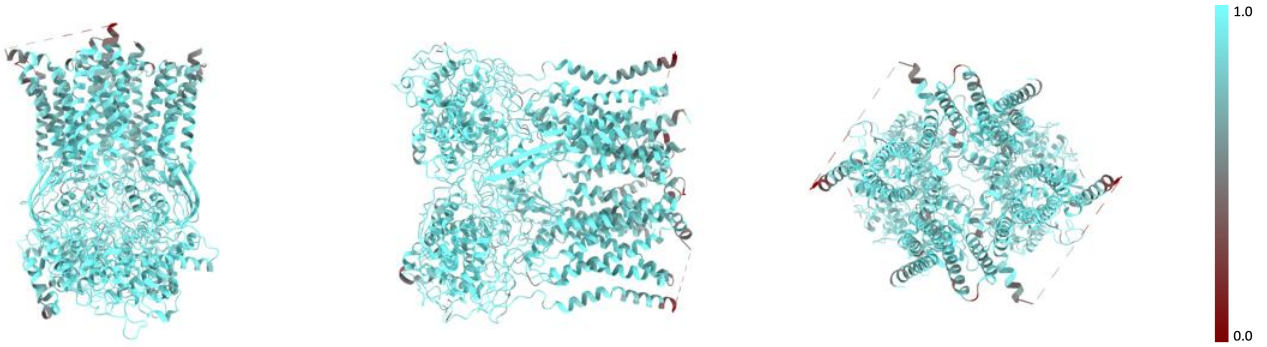
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

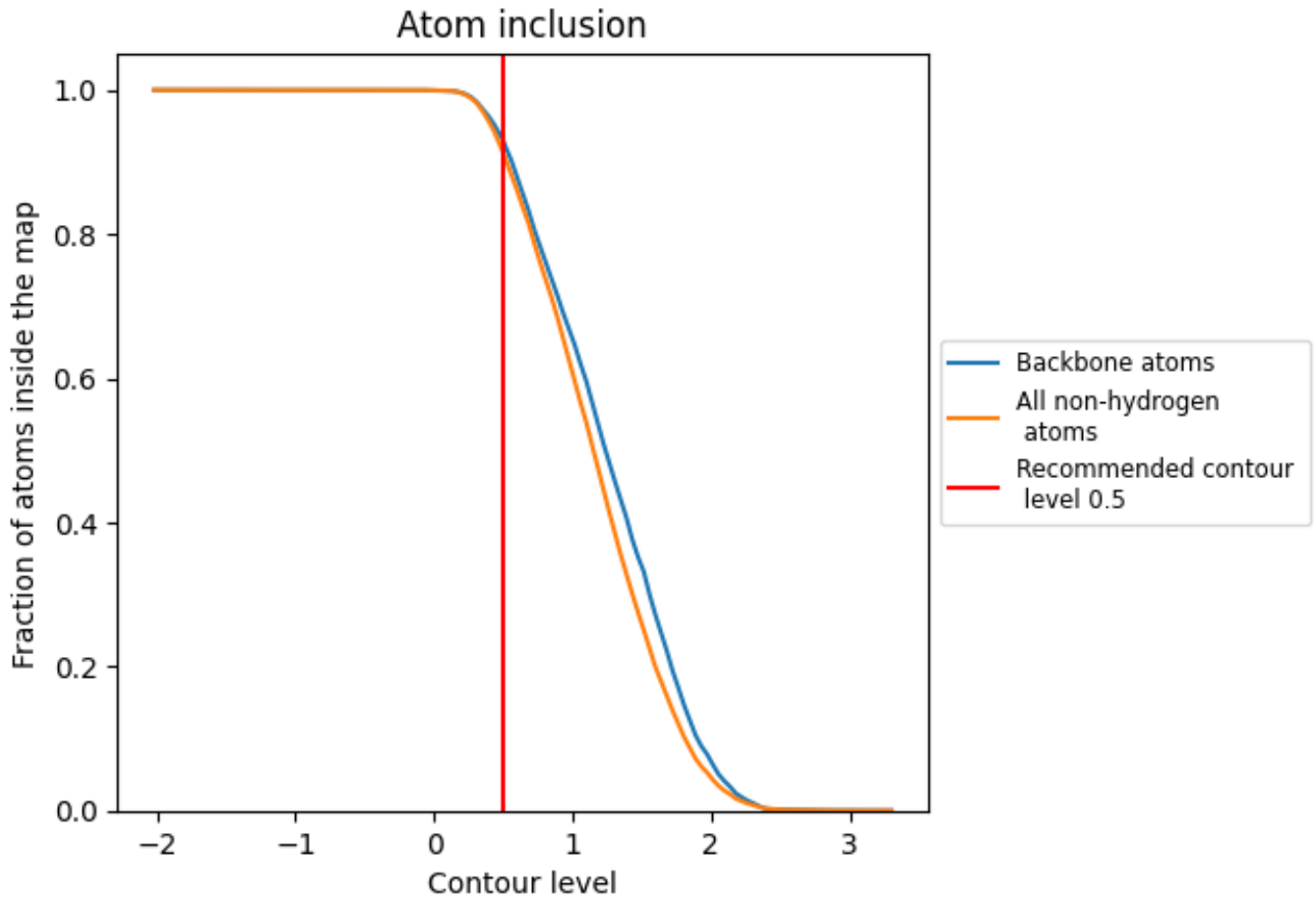
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9126	0.5940
A	0.9223	0.5980
B	0.8808	0.5810
C	0.9221	0.5990
D	0.8812	0.5820
E	0.9449	0.5950
F	0.9449	0.5940